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Comparison of simple potential functions for simulating liquid water WL Jorgensen, J Chandrasekhar, JD Madura, RW Impey, ML Klein The Journal of chemical physics 79 (2), 926-935	35806	1983
Constant pressure molecular dynamics algorithms GJ Martyna, DJ Tobias, ML Klein The Journal of chemical physics 101 (5), 4177-4189	4460	1994
Nosé–Hoover chains: The canonical ensemble via continuous dynamics GJ Martyna, ML Klein, M Tuckerman The Journal of chemical physics 97 (4), 2635-2643	4210	1992
Constant pressure molecular dynamics for molecular systems S Nosé, ML Klein Molecular Physics 50 (5), 1055-1076	2914	1983
Explicit reversible integrators for extended systems dynamics GJ Martyna, ME Tuckerman, DJ Tobias, ML Klein Molecular Physics 87 (5), 1117-1157	1926	1996
Revolutionizing science and engineering through cyberinfrastructure: Report of the National Science Foundation blue-ribbon advisory panel on cyberinfrastructure DE Atkins National Science Foundation	1142 *	2003
On the quantum nature of the shared proton in hydrogen bonds ME Tuckerman, D Marx, ML Klein, M Parrinello Science 275 (5301), 817-820	809	1997
Self-assembly of Janus dendrimers into uniform dendrimersomes and other complex architectures V Percec, DA Wilson, P Leowanawat, CJ Wilson, AD Hughes, ... Science 328 (5981), 1009-1014	674	2010

- [Using collective variables to drive molecular dynamics simulations](#) 646 2013
G Fiorin, ML Klein, J Hénin
Molecular Physics 111 (22-23), 3345-3362
- [Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional](#) 640 2016
J Sun, RC Remsing, Y Zhang, Z Sun, A Ruzsinszky, H Peng, Z Yang, ...
Nature chemistry 8 (9), 831-836
- [From molecules to materials: Current trends and future directions](#) 610 1998
P Alivisatos, PF Barbara, AW Castleman, J Chang, DA Dixon, ML Klein, ...
Advanced Materials 10 (16), 1297-1336
- [A coarse grain model for phospholipid simulations](#) 607 2001
JC Shelley, MY Shelley, RC Reeder, S Bandyopadhyay, ML Klein
The Journal of Physical Chemistry B 105 (19), 4464-4470
- [A polarizable model for water using distributed charge sites](#) 598 1988
M Sprik, ML Klein
The Journal of chemical physics 89 (12), 7556-7560
- [Coarse grain models and the computer simulation of soft materials](#) 580 2004
SO Nielsen, CF Lopez, G Srinivas, ML Klein
Journal of Physics: Condensed Matter 16 (15), R481
- [De novo design of antimicrobial polymers, foldamers, and small molecules: from discovery to practical applications](#) 553 2010
GN Tew, RW Scott, ML Klein, WF DeGrado
Accounts of chemical research 43 (1), 30-39
- [Molecular model for aqueous ferrous–ferric electron transfer](#) 550 1988
RA Kuharski, JS Bader, D Chandler, M Sprik, ML Klein, RW Impey
The Journal of chemical physics 89 (5), 3248-3257
- [Simulation of a monolayer of alkyl thiol chains](#) 548 1989
J Hautman, ML Klein
The Journal of Chemical Physics 91 (8), 4994-5001
- [De novo design of biomimetic antimicrobial polymers](#) 538 2002
GN Tew, D Liu, B Chen, RJ Doerksen, J Kaplan, PJ Carroll, ML Klein, ...
Proceedings of the National Academy of Sciences 99 (8), 5110-5114
- [Efficient molecular dynamics and hybrid Monte Carlo algorithms for path integrals](#) 524 1993
ME Tuckerman, BJ Berne, GJ Martyna, ML Klein
The Journal of Chemical Physics 99 (4), 2796-2808
- [Intermolecular potential functions and the properties of water](#) 476 1982
JR Reimers, RO Watts, ML Klein
Chemical Physics 64 (1), 95-114

- Large-scale molecular dynamics simulations of self-assembling systems** 460 2008
ML Klein, W Shinoda
Science 321 (5890), 798-800
- Multi-property fitting and parameterization of a coarse grained model for aqueous surfactants** 450 2007
W Shinoda, R DeVane, ML Klein
Molecular Simulation 33 (1-2), 27-36
- Probing the structure of DNA- carbon nanotube hybrids with molecular dynamics** 447 2008
RR Johnson, ATC Johnson, ML Klein
Nano letters 8 (1), 69-75
- Molecular-dynamics simulation of aqueous mixtures: methanol, acetone, and ammonia** 447 1990
M Ferrario, M Haughney, IR McDonald, ML Klein
The Journal of chemical physics 93 (7), 5156-5166
- Emerging applications of polymersomes in delivery: From molecular dynamics to shrinkage of tumors** 432 2007
DE Discher, V Ortiz, G Srinivas, ML Klein, Y Kim, D Christian, S Cai, ...
Progress in polymer science 32 (8-9), 838-857
- Self-assembly and properties of diblock copolymers by coarse-grain molecular dynamics** 419 2004
G Srinivas, DE Discher, ML Klein
Nature materials 3 (9), 638-644
- Liquid water from first principles: Investigation of different sampling approaches** 412 2004
IFW Kuo, CJ Mundy, MJ McGrath, JI Siepmann, J VandeVondele, M Sprik, ...
The Journal of Physical Chemistry B 108 (34), 12990-12998
- Exploring multidimensional free energy landscapes using time-dependent biases on collective variables** 408 2010
J Henin, G Fiorin, C Chipot, ML Klein
Journal of chemical theory and computation 6 (1), 35-47
- Metadynamics as a tool for exploring free energy landscapes of chemical reactions** 402 2006
B Ensing, M De Vivo, Z Liu, P Moore, ML Klein
Accounts of chemical research 39 (2), 73-81
- Rare gas solids** 401 1976
ML Klein, ML Klein, JA Venables, JA Venables
Academic Press
- Effective pair potentials and the properties of water** 384 1989

- K Watanabe, ML Klein
Chemical Physics 131 (2-3), 157-167
- Hydrogen bonding in water** 378 2003
B Chen, I Ivanov, ML Klein, M Parrinello
Physical Review Letters 91 (21), 215503
- Second-order elastic constants of a solid under stress** 371 1965
THK Barron, ML Klein
Proceedings of the Physical Society (1958-1967) 85 (3), 523
- Shrinkage of a rapidly growing tumor by drug-loaded polymersomes: pH-triggered release through copolymer degradation** 366 2006
F Ahmed, RI Pakunlu, G Srinivas, A Brannan, F Bates, ML Klein, T Minko, ...
Molecular pharmaceutics 3 (3), 340-350
- Efficient and general algorithms for path integral Car–Parrinello molecular dynamics** 362 1996
ME Tuckerman, D Marx, ML Klein, M Parrinello
The Journal of chemical physics 104 (14), 5579-5588
- Path-integral Monte Carlo study of low-temperature He 4 clusters** 349 1989
P Sindzingre, ML Klein, DM Ceperley
Physical review letters 63 (15), 1601
- X-ray diffraction and computation yield the structure of alkanethiols on gold (111)** 341 2008
A Cossaro, R Mazzarello, R Rousseau, L Casalis, A Verdini, A Kohlmeyer, ...
Science 321 (5891), 943-946
- Understanding nature's design for a nanosyringe** 341 2004
CF Lopez, SO Nielsen, PB Moore, ML Klein
Proceedings of the National Academy of Sciences 101 (13), 4431-4434
- Molecular dynamics study of the self-assembled monolayer composed of S (CH₂)₁₄CH₃ molecules using an all-atoms model** 308 1994
W Mar, ML Klein
Langmuir 10 (1), 188-196
- A recipe for the computation of the free energy barrier and the lowest free energy path of concerted reactions** 287 2005
B Ensing, A Laio, M Parrinello, ML Klein
The journal of physical chemistry B 109 (14), 6676-6687
- Pairwise additive effective potentials for nitrogen** 279 1980
CS Murthy, K Singer, ML Klein, IR McDonald
Molecular Physics 41 (6), 1387-1399
- Ab initio theory and modeling of water** 271 2017
M Chen, HY Ko, RC Remsing, MF Calegari Andrade, B Santra, Z Sun, ...

Proceedings of the National Academy of Sciences 114 (41), 10846-10851

- Superfluidity in clusters of p-H 2 molecules** 270 1991
 P Sindzingre, DM Ceperley, ML Klein
 Physical review letters 67 (14), 1871
- Nontoxic membrane-active antimicrobial arylamide oligomers** 264 2004
 D Liu, S Choi, B Chen, RJ Doerksen, DJ Clements, JD Winkler, ML Klein, ...
 Angewandte Chemie International Edition 43 (9), 1158-1162
- Constant pressure and temperature molecular dynamics simulation of a fully hydrated liquid crystal phase dipalmitoylphosphatidylcholine bilayer** 264 1995
 K Tu, DJ Tobias, ML Klein
 Biophysical journal 69 (6), 2558-2562
- Zwitterionic lipid assemblies: molecular dynamics studies of monolayers, bilayers, and vesicles using a new coarse grain force field** 259 2010
 W Shinoda, R DeVane, ML Klein
 The Journal of Physical Chemistry B 114 (20), 6836-6849
- Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus** 253 2010
 R Acharya, V Carnevale, G Fiorin, BG Levine, AL Polishchuk, V Balannik, ...
 Proceedings of the National Academy of Sciences 107 (34), 15075-15080
- Constant-pressure molecular dynamics investigation of cholesterol effects in a dipalmitoylphosphatidylcholine bilayer** 252 1998
 K Tu, ML Klein, DJ Tobias
 Biophysical journal 75 (5), 2147-2156
- Influence of a knot on the strength of a polymer strand** 246 1999
 AM Saitta, PD Soper, E Wasserman, ML Klein
 Nature 399 (6731), 46-48
- Molecular dynamics simulation of the effects of temperature on a dense monolayer of long-chain molecules** 246 1990
 J Hautman, ML Klein
 The Journal of chemical physics 93 (10), 7483-7492
- Coarse-grained molecular modeling of non-ionic surfactant self-assembly** 242 2008
 W Shinoda, R DeVane, ML Klein
 Soft Matter 4 (12), 2454-2462
- Computer simulation studies of model biological membranes** 237 2002
 L Saiz, ML Klein
 Accounts of chemical research 35 (6), 482-489
- Atomic-scale molecular dynamics simulations of lipid membranes** 232 1997
 DJ Tobias, K Tu, ML Klein
 Current opinion in colloid & interface science 2 (1), 15-26

- [Microscopic wetting phenomena](#) 230 1991
J Hautman, ML Klein
Physical review letters 67 (13), 1763
- [A study of solid and liquid carbon tetrafluoride using the constant pressure molecular dynamics technique](#) 229 1983
S Nosé, ML Klein
The Journal of Chemical Physics 78 (11), 6928-6939
- [Simulations of phospholipids using a coarse grain model](#) 228 2001
JC Shelley, MY Shelley, RC Reeder, S Bandyopadhyay, PB Moore, ...
The Journal of Physical Chemistry B 105 (40), 9785-9792
- [Staging: A sampling technique for the Monte Carlo evaluation of path integrals](#) 227 1985
M Sprik, ML Klein, D Chandler
Physical Review B 31 (7), 4234
- [Modeling the orientational ordering transition in solid fullerene \(C60\)](#) 225 1992
M Sprik, A Cheng, ML Klein
The Journal of Physical Chemistry 96 (5), 2027-2029
- [Nanoscale organization in room temperature ionic liquids: a coarse grained molecular dynamics simulation study](#) 223 2007
BL Bhargava, R Devane, ML Klein, S Balasubramanian
Soft Matter 3 (11), 1395-1400
- [Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus](#) 217 2013
J Wang, Y Wu, C Ma, G Fiorin, J Wang, LH Pinto, RA Lamb, ML Klein, ...
Proceedings of the National Academy of Sciences 110 (4), 1315-1320
- [Dissipative particle dynamics simulations of polymersomes](#) 215 2005
V Ortiz, SO Nielsen, DE Discher, ML Klein, R Lipowsky, J Shillcock
The Journal of Physical Chemistry B 109 (37), 17708-17714
- [Prediction of the phase diagram of rigid C 60 molecules](#) 211 1993
A Cheng, ML Klein, C Caccamo
Physical review letters 71 (8), 1200
- [An Ewald summation method for planar surfaces and interfaces](#) 210 1992
J Hautman, ML Klein
Molecular Physics 75 (2), 379-395
- [Molecular dynamics investigation of the structure of a fully hydrated gel-phase dipalmitoylphosphatidylcholine bilayer](#) 205 1996
K Tu, DJ Tobias, JK Blasie, ML Klein
Biophysical journal 70 (2), 595-608

- Discrimination of methylcytosine from hydroxymethylcytosine in DNA molecules** 201 2011
M Wanunu, D Cohen-Karni, RR Johnson, L Fields, J Benner, N Peterman, ...
Journal of the American Chemical Society 133 (3), 486-492
- Molecular dynamics study of a sodium octanoate micelle in aqueous solution** 201 1988
K Watanabe, M Ferrario, ML Klein
The Journal of physical chemistry 92 (3), 819-821
- Characterization of structural and dynamical behavior in monolayers of long-chain molecules using molecular-dynamics calculations** 198 1988
JP Bareman, G Cardini, ML Klein
Physical review letters 60 (21), 2152
- Structural relaxation and dynamical correlations in a molten state near the liquid–glass transition: A molecular dynamics study** 193 1990
GF Signorini, JL Barrat, ML Klein
The Journal of chemical physics 92 (2), 1294-1303
- Molecular dynamics studies of ice Ic and the structure I clathrate hydrate of methane** 192 1983
JS Tse, ML Klein, IR McDonald
The Journal of Physical Chemistry 87 (21), 4198-4203
- An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations** 190 2012
E Vargas, V Yarov-Yarovoy, F Khalili-Araghi, WA Catterall, ML Klein, ...
Journal of General Physiology 140 (6), 587-594
- Free energy landscape of a DNA– carbon nanotube hybrid using replica exchange molecular dynamics** 187 2009
RR Johnson, A Kohlmeyer, ATC Johnson, ML Klein
Nano Letters 9 (2), 537-541
- An *ab initio* study of water molecules in the bromide ion solvation shell** 187 2002
S Raugei, ML Klein
The Journal of chemical physics 116 (1), 196-202
- Hydrogen bonding structure and dynamics of water at the dimyristoylphosphatidylcholine lipid bilayer surface from a molecular dynamics simulation** 181 2004
CF Lopez, SO Nielsen, ML Klein, PB Moore
The Journal of Physical Chemistry B 108 (21), 6603-6610
- Localization and mobility of benzene in sodium-Y zeolite by molecular dynamics calculations** 180 1989
P Demontis, S Yashonath, ML Klein
The Journal of Physical Chemistry 93 (13), 5016-5019

- Energy conservation in adaptive hybrid atomistic/coarse-grain molecular dynamics** 179 2007
B Ensing, SO Nielsen, PB Moore, ML Klein, M Parrinello
Journal of Chemical Theory and Computation 3 (3), 1100-1105
- Dynamical properties of a hydrated lipid bilayer from a multianosecond molecular dynamics simulation** 178 2001
PB Moore, CF Lopez, ML Klein
Biophysical journal 81 (5), 2484-2494
- Embedded cholesterol in the nicotinic acetylcholine receptor** 176 2008
G Brannigan, J Hénin, R Law, R Eckenhoff, ML Klein
Proceedings of the National Academy of Sciences 105 (38), 14418-14423
- Intermediate states of the Kv1. 2 voltage sensor from atomistic molecular dynamics simulations** 174 2011
L Delemotte, M Tarek, ML Klein, C Amaral, W Treptow
Proceedings of the National Academy of Sciences 108 (15), 6109-6114
- Ab initio molecular dynamics simulations** 169 1996
ME Tuckerman, PJ Ungar, T Von Rosenvinge, ML Klein
The Journal of Physical Chemistry 100 (31), 12878-12887
- Collective tilt behavior in dense, substrate-supported monolayers of long-chain molecules: a molecular dynamics study** 169 1990
JP Bareman, ML Klein
Journal of Physical Chemistry 94 (13), 5202-5205
- Protonated clathrate cages enclosing neutral water molecules: $H^+(H_2O)_{21}$ and $H^+(H_2O)_{28}$** 168 2005
CC Wu, CK Lin, HC Chang, JC Jiang, JL Kuo, ML Klein
The Journal of chemical physics 122 (7), 074315
- Structural properties of a highly polyunsaturated lipid bilayer from molecular dynamics simulations** 167 2001
L Saiz, ML Klein
Biophysical journal 81 (1), 204-216
- Hydration structure of salt solutions from *ab initio* molecular dynamics** 162 2013
A Bankura, V Carnevale, ML Klein
The Journal of chemical physics 138 (1), 014501
- Molecular dynamics simulations of a protein in the canonical ensemble** 162 1993
DJ Tobias, GJ Martyna, ML Klein
The Journal of Physical Chemistry 97 (49), 12959-12966
- Nanoparticle shape improves delivery: rational coarse grain molecular dynamics (rCG-MD) of taxol in worm-like PEG-PCL micelles** 161 2012
SM Loverde, ML Klein, DE Discher

Advanced materials 24 (28), 3823-3830

Structure of hydrophilic self-assembled monolayers: A combined scanning tunneling microscopy and computer simulation study 161 1994

M Sprik, E Delamarche, B Michel, U Röthlisberger, ML Klein, H Wolf, ...
Langmuir 10 (11), 4116-4130

Membrane protein structure, function, and dynamics: a perspective from experiments and theory 159 2015

Z Cournia, TW Allen, I Andricioaei, B Antonny, D Baum, G Brannigan, ...
The Journal of membrane biology 248 (4), 611-640

Effect of Intercalated Metals on the Electrocatalytic Activity of 1T-MoS₂ for the Hydrogen Evolution Reaction 154 2017

NH Attanayake, AC Thenuwara, A Patra, YV Aulin, TM Tran, ...
ACS Energy Letters 3 (1), 7-13

Computer simulation of muonium in water 154 1984

B De Raedt, M Sprik, ML Klein
The Journal of chemical physics 80 (11), 5719-5724

Modified nonequilibrium molecular dynamics for fluid flows with energy conservation 153 1997

ME Tuckerman, CJ Mundy, S Balasubramanian, ML Klein
The Journal of chemical physics 106 (13), 5615-5621

Disorder in the pseudohexagonal rotator phase of n-alkanes: molecular-dynamics calculations for tricosane 153 1989

JP Ryckaert, IR McDonald, ML Klein
Molecular Physics 67 (5), 957-979

Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer 152 2018

M Chen, L Zheng, B Santra, HY Ko, RA DiStasio Jr, ML Klein, R Car, X Wu
Nature chemistry 10 (4), 413-419

Measurement of the Higgs boson mass from the $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4\ell$ collisions at center-of-mass energies of 7 and 8 TeV with the ATLAS detector 152 2014

M Agostoni, HP Beck, A Cervelli, A Ereditato, V Gallo, S Haug, T Kruker, ...
Physical review. D-particles, fields, gravitation, and cosmology 90 (5), 052004

Molecular dynamics studies of the structure of water at high temperatures and density 152 1981

RW Impey, ML Klein, IR McDonald
The Journal of Chemical Physics 74 (1), 647-652

Solvent polarization and hydration of the chlorine anion 151 1990

M Sprik, ML Klein, K Watanabe

Journal of Physical Chemistry 94 (16), 6483-6488

Molecular dynamics calculations for the liquid and cubic plastic crystal phases of carbon tetrachloride 149 1982

IR McDonald, DG Bounds, ML Klein
Molecular Physics 45 (3), 521-542

Structure, dynamics, and spectral diffusion of water from first-principles molecular dynamics 147 2014

A Bankura, A Karmakar, V Carnevale, A Chandra, ML Klein
The Journal of Physical Chemistry C 118 (50), 29401-29411

A coarse grain model for *n*-alkanes parameterized from surface tension data 147 2003

SO Nielsen, CF Lopez, G Srinivas, ML Klein
The Journal of chemical physics 119 (14), 7043-7049

Molecular dynamics investigations of self-assembled monolayers 147 1991

J Hautman, JP Bareman, W Mar, ML Klein
Journal of the Chemical Society, Faraday Transactions 87 (13), 2031-2037

Computer simulation studies of the structure I clathrate hydrates of methane, tetrafluoromethane, cyclopropane, and ethylene oxide 146 1984

JS Tse, ML Klein, IR McDonald
The Journal of chemical physics 81 (12), 6146-6153

Molecular dynamics simulation directed rational design of inhibitors targeting drug-resistant mutants of influenza A virus M2 145 2011

J Wang, C Ma, G Fiorin, V Carnevale, T Wang, F Hu, RA Lamb, LH Pinto, ...
Journal of the American Chemical Society 133 (32), 12834-12841

Molecular dynamics simulation of tetradecyltrimethylammonium bromide monolayers at the air/water interface 143 1995

M Tarek, DJ Tobias, ML Klein
The Journal of Physical Chemistry 99 (5), 1393-1402

Molecular-dynamics investigation of orientational freezing in solid C 60 140 1992

A Cheng, ML Klein
Physical Review B 45 (4), 1889

Calculation of infrared intensities by the CNDO method 140 1967

GA Segal, ML Klein
The Journal of Chemical Physics 47 (10), 4236-4240

Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium 139 2001

B Chen, JI Siepmann, KJ Oh, ML Klein
The Journal of chemical physics 115 (23), 10903-10913

Pressure-induced phase transformations in ice 139 1987

ST John, ML Klein

Physical review letters 58 (16), 1672

- Molecular dynamics simulation of an aqueous sodium octanoate micelle using polarizable surfactant molecules** 138 1993
JC Shelley, M Sprik, ML Klein
Langmuir 9 (4), 916-926
- Self-assembly of amphiphilic Janus dendrimers into uniform onion-like dendrimersomes with predictable size and number of bilayers** 137 2014
S Zhang, HJ Sun, AD Hughes, RO Moussodia, A Bertin, Y Chen, ...
Proceedings of the National Academy of Sciences 111 (25), 9058-9063
- Phosphodiester cleavage in ribonuclease H occurs via an associative two-metal-aided catalytic mechanism** 137 2008
M De Vivo, M Dal Peraro, ML Klein
Journal of the American Chemical Society 130 (33), 10955-10962
- Simulation of a sodium dodecylsulfate micelle in aqueous solution** 136 1990
J Shelley, K Watanabe, ML Klein
International Journal of Quantum Chemistry 38 (S17), 103-117
- Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units** 135 2012
DN LeBard, BG Levine, P Mertmann, SA Barr, A Jusufi, S Sanders, ...
Soft Matter 8 (8), 2385-2397
- Quantum nuclear *ab initio* molecular dynamics study of water wires** 134 1998
HS Mei, ME Tuckerman, DE Sagnella, ML Klein
The Journal of Physical Chemistry B 102 (50), 10446-10458
- An *ab initio* path integral molecular dynamics study of double proton transfer in the formic acid dimer** 134 1998
S Miura, ME Tuckerman, ML Klein
The Journal of chemical physics 109 (13), 5290-5299
- Molecular dynamics study of a lipid- DNA complex** 133 1999
S Bandyopadhyay, M Tarek, ML Klein
The Journal of Physical Chemistry B 103 (46), 10075-10080
- Multiple binding sites for the general anesthetic isoflurane identified in the nicotinic acetylcholine receptor transmembrane domain** 132 2010
G Brannigan, DN LeBard, J Hénin, RG Eckenhoff, ML Klein
Proceedings of the National Academy of Sciences 107 (32), 14122-14127
- Polytypism and the vibrational properties of PbI_2** 132 1979
WM Sears, ML Klein, JA Morrison
Physical Review B 19 (4), 2305
- The nature of DNA-base-carbon-nanotube interactions** 131 2010
RR Johnson, ATC Johnson, ML Klein

small 6 (1), 31-34

- Transferable coarse grain nonbonded interaction model for amino acids** 130 2009
R DeVane, W Shinoda, PB Moore, ML Klein
Journal of chemical Theory and Computation 5 (8), 2115-2124
- An improved self-consistent phonon approximation** 128 1968
VV Goldman, GK Horton, ML Klein
Physical Review Letters 21 (22), 1527
- Molecular dynamics calculations suggest a conduction mechanism for the M2 proton channel from influenza A virus** 127 2009
E Khurana, MD Peraro, R DeVane, S Vemparala, WF DeGrado, ML Klein
Proceedings of the National Academy of Sciences 106 (4), 1069-1074
- Diabatic free energy curves and coordination fluctuations for the aqueous Ag^+ / Ag^{2+} redox couple: A biased Born-Oppenheimer molecular dynamics investigation** 127 2006
J Blumberger, I Tavernelli, ML Klein, M Sprik
The Journal of chemical physics 124 (6), 064507
- Distribution of halothane in a dipalmitoylphosphatidylcholine bilayer from molecular dynamics calculations** 127 2000
L Koubi, M Tarek, ML Klein, D Scharf
Biophysical journal 78 (2), 800-811
- A molecular dynamics study of methane in zeolite NaY** 126 1988
S Yashonath, P Demontis, ML Klein
Chemical physics letters 153 (6), 551-556
- Understanding TRPV1 activation by ligands: Insights from the binding modes of capsaicin and resiniferatoxin** 124 2016
K Elokely, P Velisetty, L Delemotte, E Palovcak, ML Klein, T Rohacs, ...
Proceedings of the National Academy of Sciences 113 (2), E137-E145
- Translational and rotational disorder in solid *n*-alkanes: Constant temperature–constant pressure molecular dynamics calculations using infinitely long flexible chains** 124 1986
JP Ryckaert, ML Klein
The Journal of chemical physics 85 (3), 1613-1620
- Structure and dynamics of associated molecular systems. I. Computer simulation of liquid hydrogen fluoride** 124 1979
ML Klein, IR McDonald
The Journal of Chemical Physics 71 (1), 298-308
- Modelling room temperature ionic liquids** 122 2008
BL Bhargava, S Balasubramanian, ML Klein
Chemical communications, 3339-3351

- Structural transformations in solid nitrogen at high pressure** 122 1983
S Nosé, ML Klein
Physical Review Letters 50 (16), 1207
- Structure of water at charged interfaces: A molecular dynamics study** 121 2014
S Dewan, V Carnevale, A Bankura, A Eftekhari-Bafrooei, G Fiorin, ...
Langmuir 30 (27), 8056-8065
- Computer simulation studies of biomembranes using a coarse grain model** 121 2002
CF Lopez, PB Moore, JC Shelley, MY Shelley, ML Klein
Computer Physics Communications 147 (1-2), 1-6
- Molecular dynamics simulations of a calcium carbonate/calcium sulfonate reverse micelle** 121 1996
DJ Tobias, ML Klein
The Journal of Physical Chemistry 100 (16), 6637-6648
- Effect of interlayer spacing on the activity of layered manganese oxide bilayer catalysts for the oxygen evolution reaction** 119 2017
Q Kang, L Vernisse, RC Remsing, AC Thenuwara, SL Shumlas, ...
Journal of the American Chemical Society 139 (5), 1863-1870
- Effects of anesthetics on the structure of a phospholipid bilayer: molecular dynamics investigation of halothane in the hydrated liquid crystal phase of ...** 119 1998
K Tu, M Tarek, ML Klein, D Scharf
Biophysical journal 75 (5), 2123-2134
- Catalytic metal ions and enzymatic processing of DNA and RNA** 118 2015
G Palermo, A Cavalli, ML Klein, M Alfonso-Prieto, M Dal Peraro, ...
Accounts of chemical research 48 (2), 220-228
- Ab initio molecular dynamics study of proton transfer in a polyglycine analog of the ion channel gramicidin A** 118 1996
DE Sagnella, K Laasonen, ML Klein
Biophysical journal 71 (3), 1172-1178
- Molecular dynamics simulations of supercooled liquids near the glass transition** 118 1991
JL Barrat, JN Roux
Journal of non-crystalline solids 131, 255-261
- Functional studies and modeling of pore-lining residue mutants of the influenza A virus M2 ion channel** 117 2010
V Balannik, V Carnevale, G Fiorin, BG Levine, RA Lamb, ML Klein, ...
Biochemistry 49 (4), 696-708
- Nickel confined in the interlayer region of birnessite: an active electrocatalyst for water oxidation** 115 2016
AC Thenuwara, EB Cerkez, SL Shumlas, NH Attanayake, IG McKendry, ...

Angewandte Chemie 128 (35), 10537-10541

Hydrogen-bond topology and the ice VII/VIII and ice I h/XI proton-ordering phase transitions 114 2005

SJ Singer, JL Kuo, TK Hirsch, C Knight, L Ojamäe, ML Klein
Physical review letters 94 (13), 135701

Thermodynamic properties of solid Ar, Kr, and Xe based upon a short-range central force and the conventional perturbation expansion of the partition function 113 1969

ML Klein, GK Horton, JL Feldman
Physical Review 184 (3), 968

Orientational ordering in solid C 70: Predictions from computer simulation 112 1992

M Sprik, A Cheng, ML Klein
Physical review letters 69 (11), 1660

Mimicking biological membranes with programmable glycan ligands self-assembled from amphiphilic Janus glycodendrimers 111 2014

S Zhang, RO Moussodia, HJ Sun, P Leowanawat, A Muncan, ...
Angewandte Chemie 126 (41), 11079-11083

Structure of protonated water clusters: Low-energy structures and finite temperature behavior 111 2005

JL Kuo, ML Klein
The Journal of chemical physics 122 (2), 024516

Molecular dynamics simulations of solid buckminsterfullerenes 111 1991

A Cheng, ML Klein
The Journal of Physical Chemistry 95 (18), 6750-6751

Computer simulation studies of solids 111 1985

ML Klein
Annual Review of Physical Chemistry 36 (1), 525-548

Discovery of novel dual inhibitors of the wild-type and the most prevalent drug-resistant mutant, S31N, of the M2 proton channel from influenza A virus 110 2013

J Wang, C Ma, J Wang, H Jo, B Canturk, G Fiorin, LH Pinto, RA Lamb, ...
Journal of medicinal chemistry 56 (7), 2804-2812

Computer simulation studies of self-assembling macromolecules 110 2012

W Shinoda, R DeVane, ML Klein
Current opinion in structural biology 22 (2), 175-186

Simulation of diblock copolymer self-assembly, using a coarse-grain model 110 2004

G Srinivas, JC Shelley, SO Nielsen, DE Discher, ML Klein
The Journal of Physical Chemistry B 108 (24), 8153-8160

The effects of pressure on structural and dynamical properties of associated 110 1997

- liquids: Molecular dynamics calculations for the extended simple point charge model of water**
K Bagchi, S Balasubramanian, ML Klein
The Journal of chemical physics 107 (20), 8561-8567
- Calculation of the shear viscosity of decane using a reversible multiple time-step algorithm** 110 1995
CJ Mundy, JI Siepmann, ML Klein
The Journal of chemical physics 102 (8), 3376-3380
- Optimization of a distributed Gaussian basis set using simulated annealing: application to the adiabatic dynamics of the solvated electron** 110 1988
M Sprik, ML Klein
The Journal of chemical physics 89 (3), 1592-1607
- Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations** 110 1985
M Sprik, RW Impey, ML Klein
The Journal of chemical physics 83 (11), 5802-5809
- Second-order elastic constants for the Lennard-Jones solid** 110 1984
M Sprik, RW Impey, ML Klein
Physical Review B 29 (8), 4368
- Solvation Structure and Mobility Mechanism of OH⁻: A Car-Parrinello Molecular Dynamics Investigation of Alkaline Solutions** 108 2002
B Chen, I Ivanov, JM Park, M Parrinello, ML Klein
The Journal of Physical Chemistry B 106 (46), 12006-12016
- Direct Gibbs ensemble Monte Carlo simulations for solid-vapor phase equilibria: applications to Lennard-Jonesium and carbon dioxide** 108 2001
B Chen, JI Siepmann, ML Klein
The Journal of Physical Chemistry B 105 (40), 9840-9848
- Rare Gas Solids** 108 * 1976
MLKJA Venables
Academic Press
- Disorder at the bilayer interface in the pseudo-hexagonal rotator phase of solid n-alkanes** 106 1987
JP Ryckaert, ML Klein, IR McDonald
Physical review letters 58 (7), 698
- A simple intermolecular potential for liquid ammonia** 106 1984
RW Impey, ML Klein
Chemical physics letters 104 (6), 579-582
- Unfolding a linker between helical repeats** 105 2005
V Ortiz, SO Nielsen, ML Klein, DE Discher
Journal of molecular biology 349 (3), 638-647

- Electrostatic interactions in a neutral model phospholipid bilayer by molecular dynamics simulations** 105 2002
L Saiz, ML Klein
The Journal of chemical physics 116 (7), 3052-3057
- Computational studies of room temperature ionic liquid–water mixtures** 104 2011
BL Bhargava, Y Yasaka, ML Klein
Chemical Communications 47 (22), 6228-6241
- Surfactant aggregation at a hydrophobic surface** 104 1998
S Bandyopadhyay, JC Shelley, M Tarek, PB Moore, ML Klein
The Journal of Physical Chemistry B 102 (33), 6318-6322
- Molecular dynamics simulation of a synthetic ion channel** 104 1998
Q Zhong, Q Jiang, PB Moore, DM Newns, ML Klein
Biophysical journal 74 (1), 3-10
- Shape fluctuations in ionic micelles** 103 1989
K Watanabe, ML Klein
The Journal of Physical Chemistry 93 (19), 6897-6901
- Towards an understanding of complex biological membranes from atomistic molecular dynamics simulations** 102 2002
L Saiz, S Bandyopadhyay, ML Klein
Bioscience reports 22 (2), 151-173
- Role of zinc content on the catalytic efficiency of B1 metallo β -lactamases** 101 2007
M Dal Peraro, AJ Vila, P Carloni, ML Klein
Journal of the American Chemical Society 129 (10), 2808-2816
- Lipid bilayer perturbations around a transmembrane nanotube: a coarse grain molecular dynamics study** 101 2005
SO Nielsen, B Ensing, V Ortiz, PB Moore, ML Klein
Biophysical Journal 88 (6), 3822-3828
- Ab initio molecular dynamics study of hydrochloric acid in water** 101 1994
K Laasonen, ML Klein
Journal of the American Chemical Society 116 (25), 11620-11621
- The M2 channel of influenza A virus: a molecular dynamics study** 100 1998
Q Zhong, T Husslein, PB Moore, DM Newns, P Pattnaik, ML Klein
Febs Letters 434 (3), 265-271
- Biomimetic facially amphiphilic antibacterial oligomers with conformationally stiff backbones** 99 2006
H Tang, RJ Doerksen, TV Jones, ML Klein, GN Tew
Chemistry & biology 13 (4), 427-435

- Neon interatomic potentials from scattering data and crystalline properties** 99 1973
JM Farrar, YT Lee, VV Goldman, ML Klein
Chemical Physics Letters 19 (3), 359-362
- Vapor– Liquid interfacial properties of mutually saturated water/1-butanol solutions** 98 2002
B Chen, JI Siepmann, ML Klein
Journal of the American Chemical Society 124 (41), 12232-12237
- Ionic solvation in nonaqueous solvents: the structure of lithium ion and chloride in methanol, ammonia, and methylamine** 97 1987
RW Impey, M Sprik, ML Klein
Journal of the American Chemical Society 109 (20), 5900-5904
- Key roles for chain flexibility in block copolymer membranes that contain pores or make tubes** 96 2005
G Srinivas, DE Discher, ML Klein
Nano letters 5 (12), 2343-2349
- A molecular dynamics study of methanol near the liquid–glass transition** 96 1992
P Sindzingre, ML Klein
The Journal of chemical physics 96 (6), 4681-4692
- Simulation of an excess electron in a hard sphere fluid** 96 1985
M Sprik, ML Klein, D Chandler
The Journal of chemical physics 83 (6), 3042-3049
- Polarization effects and charge transfer in the KcsA potassium channel** 95 2006
D Bucher, S Raugei, L Guidoni, M Dal Peraro, U Rothlisberger, P Carloni, ...
Biophysical chemistry 124 (3), 292-301
- Molecular Dynamics Simulations of Surfactant Self-Organization at a Solid–Liquid Interface** 95 2006
G Srinivas, SO Nielsen, PB Moore, ML Klein
Journal of the American Chemical Society 128 (3), 848-853
- An intermolecular force model for (HF)₂** 94 1978
ML Klein, IR McDonald, SF O'Shea
The Journal of Chemical Physics 69 (1), 63-66
- Solute–solvent charge transfer in aqueous solution** 93 2005
M Dal Peraro, S Raugei, P Carloni, ML Klein
ChemPhysChem 6 (9), 1715-1718
- Structural study of (H₂O)₂₀ and (H₂O)₂₁H⁺ using density functional methods** 93 1994
K Laasonen, ML Klein
The Journal of Physical Chemistry 98 (40), 10079-10083
- Characterization of nonbiological antimicrobial polymers in aqueous solution** 92 2006

and at water– lipid interfaces from all-atom molecular dynamics

I Ivanov, S Vemparala, V Pophristic, K Kuroda, WF DeGrado, ...
Journal of the American Chemical Society 128 (6), 1778-1779

Elastic constants and phonon dispersion curves for solid argon near 0 K

JA Barker, ML Klein, MV Bobetic
Physical Review B 2 (10), 4176

92 1970

First-principles study of aqueous hydroxide solutions

B Chen, JM Park, I Ivanov, G Tabacchi, ML Klein, M Parrinello
Journal of the American Chemical Society 124 (29), 8534-8535

91 2002

Exploration of the structural features defining the conduction properties of a synthetic ion channel

GR Dieckmann, JD Lear, Q Zhong, ML Klein, WF DeGrado, KA Sharp
Biophysical Journal 76 (2), 618-630

91 1999

Path-integral Monte Carlo studies of *para*-hydrogen clusters

D Scharf, ML Klein, GJ Martyna
The Journal of chemical physics 97 (5), 3590-3599

91 1992

United-atom acyl chains for CHARMM phospholipids

J Hénin, W Shinoda, ML Klein
The Journal of Physical Chemistry B 112 (23), 7008-7015

90 2008

Shear viscosity of polar fluids: Molecular dynamics calculations of water

S Balasubramanian, CJ Mundy, ML Klein
The Journal of chemical physics 105 (24), 11190-11195

90 1996

Perspective on the reactions between F–and CH₃CH₂F: The free energy landscape of the E2 and SN₂ reaction channels

B Ensing, ML Klein
Proceedings of the National Academy of Sciences 102 (19), 6755-6759

89 2005

Vibrational predissociation spectra and hydrogen-bond topologies of H+(H₂O) 9–11

CK Lin, CC Wu, YS Wang, YT Lee, HC Chang, JL Kuo, ML Klein
Physical Chemistry Chemical Physics 7 (5), 938-944

89 2005

Dynamical structure factor $S(Q \rightarrow, \omega)$ of rare-gas solids

JP Hansen, ML Klein
Physical Review B 13 (2), 878

89 1976

Dissecting molecular aspects of cell interactions using glycodendrimerosomes with programmable glycan presentation and engineered human lectins

S Zhang, RO Moussodia, C Murzeau, HJ Sun, ML Klein, S Vértesy, ...
Angewandte Chemie 127 (13), 4108-4112

88 2015

- A minimum free energy reaction path for the E2 reaction between fluoroethane and a fluoride ion** 88 2004
B Ensing, A Laio, FL Gervasio, M Parrinello, ML Klein
Journal of the American Chemical Society 126 (31), 9492-9493
- Lattice dynamics with three-body forces: solid Xe and Kr** 88 1976
JA Barker, ML Klein, MV Bobetic
IBM Journal of Research and Development 20 (3), 222-227
- High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction** 87 2015
JL Thomaston, M Alfonso-Prieto, RA Woldeyes, JS Fraser, ML Klein, ...
Proceedings of the National Academy of Sciences 112 (46), 14260-14265
- The design and evaluation of heparin-binding foldamers** 87 2005
S Choi, DJ Clements, V Pophristic, I Ivanov, S Vemparala, JS Bennett, ...
Angewandte Chemie International Edition 44 (41), 6685-6689
- Centroid path integral molecular dynamics simulation of lithium para-hydrogen clusters** 87 1997
K Kinugawa, PB Moore, ML Klein
The Journal of chemical physics 106 (3), 1154-1169
- Structure and dynamics of carbon dioxide clusters: a molecular dynamics study** 86 1989
G Cardini, V Schettino, ML Klein
The Journal of chemical physics 90 (8), 4441-4449
- A unitary anesthetic binding site at high resolution** 85 2009
LS Vedula, G Brannigan, NJ Economou, J Xi, MA Hall, R Liu, MJ Rossi, ...
Journal of Biological Chemistry 284 (36), 24176-24184
- Path-integral Monte Carlo study of a lithium impurity in *para*-hydrogen: Clusters and the bulk liquid** 85 1993
D Scharf, GJ Martyna, ML Klein
The Journal of chemical physics 99 (11), 8997-9012
- Anharmonic effects and the lattice dynamics of insulators** 85 1971
HR Clyde, ML Klein
Critical Reviews in Solid State and Material Sciences 2 (2), 181-254
- The torsional potential of perfluoro *n*-alkanes: A density functional study** 84 1996
U Röthlisberger, K Laasonen, ML Klein, M Sprik
The Journal of chemical physics 104 (10), 3692-3700
- Partitioning of anesthetics into a lipid bilayer and their interaction with membrane-bound peptide bundles** 83 2006
S Vemparala, L Saiz, RG Eckenhoff, ML Klein
Biophysical journal 91 (8), 2815-2825

- Molecular dynamics study of the poly (oxyethylene) surfactant C12E2 and water** 83 2000
S Bandyopadhyay, M Tarek, ML Lynch, ML Klein
Langmuir 16 (3), 942-946
- Monte Carlo calculations for solid CO and N2 overlayers physisorbed on graphite** 83 1985
C Peters, ML Klein
Molecular Physics 54 (4), 895-909
- Probing membrane insertion activity of antimicrobial polymers via coarse-grain molecular dynamics** 81 2006
CF Lopez, SO Nielsen, G Srinivas, WF DeGrado, ML Klein
Journal of chemical theory and computation 2 (3), 649-655
- Ab initio study of aqueous hydrochloric acid** 81 1997
KE Laasonen, ML Klein
The Journal of Physical Chemistry A 101 (1), 98-102
- An intermolecular potential for methane** 81 1981
R Righini, K Maki, ML Klein
Chemical Physics Letters 80 (2), 301-305
- Characterization of a Langmuir-Blodgett monolayer using molecular dynamics calculations** 80 1988
G Cardini, JP Bareman, ML Klein
Chemical physics letters 145 (6), 493-498
- Dynamical properties of the structure I clathrate hydrate of xenon^a)** 80 1983
JS Tse, ML Klein, IR McDonald
The Journal of chemical physics 78 (4), 2096-2097
- Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion** 79 2011
JE Donald, Y Zhang, G Fiorin, V Carnevale, DR Slochower, F Gai, ...
Proceedings of the National Academy of Sciences 108 (10), 3958-3963
- Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions** 79 2006
C Knight, SJ Singer, JL Kuo, TK Hirsch, L Ojamäe, ML Klein
Physical Review E 73 (5), 056113
- Micellization studied by GPU-accelerated coarse-grained molecular dynamics** 78 2011
BG Levine, DN LeBard, R DeVane, W Shinoda, A Kohlmeyer, ML Klein
Journal of Chemical Theory and Computation 7 (12), 4135-4145
- Simulation of the HIV-1 Vpu transmembrane domain as a pentameric bundle** 78 1998
PB Moore, Q Zhong, T Husslein, ML Klein
FEBS letters 431 (2), 143-148

- Orientational phases of classical quadrupoles on a triangular net** 78 1979
SF O'Shea, ML Klein
Chemical Physics Letters 66 (2), 381-383
- Flipping in the pore: discovery of dual inhibitors that bind in different orientations to the wild-type versus the amantadine-resistant S31N mutant of the influenza A virus M2 ...** 77 2014
Y Wu, B Canturk, H Jo, C Ma, E Gianti, ML Klein, LH Pinto, RA Lamb, ...
Journal of the American Chemical Society 136 (52), 17987-17995
- DNA-decorated carbon nanotubes for chemical sensing** 77 2006
ATC Johnson, C Staii, M Chen, S Khamis, R Johnson, ML Klein, ...
Semiconductor science and technology 21 (11), S17
- Equilibrium and non-equilibrium simulation studies of fluid alkanes in bulk and at interfaces** 77 1996
J IljaáSiepmann
Faraday Discussions 104, 17-36
- Glycodendrimersomes from sequence-defined Janus glycodendrimers reveal high activity and sensor capacity for the agglutination by natural variants of human lectins** 76 2015
S Zhang, Q Xiao, SE Sherman, A Muncan, ADM Ramos Vicente, Z Wang, ...
Journal of the American Chemical Society 137 (41), 13334-13344
- Exploring volatile general anesthetic binding to a closed membrane-bound bacterial voltage-gated sodium channel via computation** 76 2013
SG Raju, AF Barber, DN LeBard, ML Klein, V Carnevale
PLoS computational biology 9 (6), e1003090
- Simulating vapor- liquid nucleation of water: a combined histogram-reweighting and aggregation-volume-bias Monte Carlo investigation for fixed-charge and polarizable models** 76 2005
B Chen, JI Siepmann, ML Klein
The Journal of Physical Chemistry A 109 (6), 1137-1145
- Electronic states in metal-ammonia solutions** 76 1993
Z Deng, GJ Martyna, ML Klein
Physical review letters 71 (2), 267
- New high-pressure phases of ice** 76 1988
P Demontis, R LeSar, ML Klein
Physical review letters 60 (22), 2284
- Intermolecular potentials for ammonia based on SCF-MO calculations** 76 1981
A Hinchliffe, DG Bounds, ML Klein, IR McDonald, R Righini
The Journal of Chemical Physics 74 (2), 1211-1216

- Peptide hydrolysis in thermolysin: Ab initio QM/MM investigation of the Glu143-assisted water addition mechanism** 75 2007
J Blumberger, G Lamoureux, ML Klein
Journal of Chemical Theory and Computation 3 (5), 1837-1850
- Electron-ion interactions and ionization in a polar solvent** 74 1986
M Sprik, RW Impey, ML Klein
Physical review letters 56 (21), 2326
- Dynamical properties of solids** 74 1974
THK Barron, ML Klein
North-Holland, Amsterdam
- Self-sorting and coassembly of fluorinated, hydrogenated, and hybrid Janus dendrimers into dendrimersomes** 73 2016
Q Xiao, JD Rubien, Z Wang, EH Reed, DA Hammer, D Sahoo, PA Heiney, ...
Journal of the American Chemical Society 138 (38), 12655-12663
- Onion-like glycodendrimersomes from sequence-defined Janus glycodendrimers and influence of architecture on reactivity to a lectin** 73 2016
Q Xiao, S Zhang, Z Wang, SE Sherman, RO Moussodia, M Peterca, ...
Proceedings of the National Academy of Sciences 113 (5), 1162-1167
- Gating pore currents and the resting state of Nav1.4 voltage sensor domains** 73 2012
P Gosselin-Badaroudine, L Delemotte, A Moreau, ML Klein, M Chahine
Proceedings of the National Academy of Sciences 109 (47), 19250-19255
- Molecular dynamics investigations of lipid Langmuir monolayers using a coarse-grain model** 73 2003
SO Nielsen, CF Lopez, PB Moore, JC Shelley, ML Klein
The Journal of Physical Chemistry B 107 (50), 13911-13917
- Simulating vapor-liquid nucleation of *n*-alkanes** 73 2002
B Chen, JI Siepmann, KJ Oh, ML Klein
The Journal of chemical physics 116 (10), 4317-4329
- Monte Carlo investigations of hexadecane films on a metal substrate** 73 1995
S Balasubramanian, ML Klein, JI Siepmann
The Journal of chemical physics 103 (8), 3184-3195
- Deprotonation of a histidine residue in aqueous solution using constrained ab initio molecular dynamics** 72 2002
I Ivanov, ML Klein
Journal of the American Chemical Society 124 (45), 13380-13381
- Decane under shear: A molecular dynamics study using reversible NVT-SLLOD and NPT-SLLOD algorithms** 72 1995
CJ Mundy, JI Siepmann, ML Klein
The Journal of chemical physics 103 (23), 10192-10200

- Molecular dynamics investigation of the surface/bulk equilibrium in an ethanol–water solution** 71 1996
M Tarek, DJ Tobias, ML Klein
Journal of the Chemical Society, Faraday Transactions 92 (4), 559-563
- Temperature and concentration dependence of adsorption properties of methane in NaY: a molecular dynamics study** 71 1991
S Yashonath, P Demontis, ML Klein
The Journal of Physical Chemistry 95 (15), 5881-5889
- The rise of self-consistent phonon theory** 71 1972
ML Klein, GK Horton
Journal of Low Temperature Physics 9 (3), 151-166
- Structure and dynamics of model pore insertion into a membrane** 70 2005
CF Lopez, SO Nielsen, B Ensing, PB Moore, ML Klein
Biophysical journal 88 (5), 3083-3094
- Concentration effects of volatile anesthetics on the properties of model membranes: a coarse-grain approach** 70 2005
M Pickholz, L Saiz, ML Klein
Biophysical journal 88 (3), 1524-1534
- Nuclear quantum effects and hydrogen bonding in liquids** 70 2003
S Raugei, ML Klein
Journal of the American Chemical Society 125 (30), 8992-8993
- Membrane structural perturbations caused by anesthetics and nonimmobilizers: a molecular dynamics investigation** 70 2001
L Koubi, M Tarek, S Bandyopadhyay, ML Klein, D Scharf
Biophysical Journal 81 (6), 3339-3345
- Constant pressure and temperature molecular-dynamics simulation of the hydrated diphtanolphosphatidylcholine lipid bilayer** 70 1998
T Husslein, DM Newns, PC Pattnaik, Q Zhong, PB Moore, ML Klein
The Journal of chemical physics 109 (7), 2826-2832
- An *ab initio* molecular orbital study of NaCN and KCN** 70 1981
ML Klein, JD Goddard, DG Bounds
The Journal of Chemical Physics 75 (8), 3909-3915
- Determination of the interatomic potential of krypton** 70 1973
U Buck, MG Dondi, U Valbusa, ML Klein, G Scoles
Physical Review A 8 (5), 2409
- General anesthetics predicted to block the GLIC pore with micromolar affinity** 69 2012
DN LeBard, J Hénin, RG Eckenhoff, ML Klein, G Brannigan

PLoS computational biology 8 (5), e1002532

- Formamide hydrolysis in alkaline aqueous solution: Insight from ab initio metadynamics calculations** 69 2006
 J Blumberger, B Ensing, ML Klein
 Angewandte Chemie 118 (18), 2959-2963
- Thermodynamic properties for a simple model of solid carbon dioxide: Monte Carlo, cell model, and quasiharmonic calculations** 69 1974
 TG Gibbons, ML Klein
 The Journal of Chemical Physics 60 (1), 112-126
- Unraveling functional significance of natural variations of a human galectin by glycodendrimersomes with programmable glycan surface** 68 2015
 S Zhang, RO Moussodia, S Vértesy, S André, ML Klein, HJ Gabius, ...
 Proceedings of the National Academy of Sciences 112 (18), 5585-5590
- Pore waters regulate ion permeation in a calcium release-activated calcium channel** 68 2013
 H Dong, G Fiorin, V Carnevale, W Treptow, ML Klein
 Proceedings of the National Academy of Sciences 110 (43), 17332-17337
- Reorganization free energies for long-range electron transfer in a porphyrin-binding four-helix bundle protein** 68 2006
 J Blumberger, ML Klein
 Journal of the American Chemical Society 128 (42), 13854-13867
- Dynamics of Water Molecules in the Br⁻ Solvation Shell: An ab Initio Molecular Dynamics Study** 68 2001
 S Raugei, ML Klein
 Journal of the American Chemical Society 123 (38), 9484-9485
- C12E2 reverse micelle: A molecular dynamics study** 68 2000
 R Allen, S Bandyopadhyay, ML Klein
 Langmuir 16 (26), 10547-10552
- Thermoelastic properties of some cubic close-packed lattices** 68 1965
 THK Barron, ML Klein
 Proceedings of the Physical Society (1958-1967) 85 (3), 533
- Bioactive cell-like hybrids coassembled from (glyco) dendrimersomes with bacterial membranes** 67 2016
 Q Xiao, SS Yadavalli, S Zhang, SE Sherman, E Fiorin, L Da Silva, ...
 Proceedings of the National Academy of Sciences 113 (9), E1134-E1141
- Curvature-driven molecular demixing in the budding and breakup of mixed component worm-like micelles** 66 2010
 SM Loverde, V Ortiz, RD Kamien, ML Klein, DE Discher
 Soft Matter 6 (7), 1419-1425

- Conformational changes and gating at the selectivity filter of potassium channels** 66 2008
C Domene, ML Klein, D Branduardi, FL Gervasio, M Parrinello
Journal of the American Chemical Society 130 (29), 9474-9480
- Structure of physisorbed overlayers of dipolar molecules: A combined study by atomic-beam scattering and molecular dynamics** 66 1988
JC Ruiz-Suarez, ML Klein, MA Moller, PA Rowntree, G Scoles, J Xu
Physical review letters 61 (6), 710
- Molecular Dynamics Studies of Cation Aggregation in the Room Temperature Ionic Liquid [C₁₀mim][Br] in Aqueous Solution** 65 2009
BL Bhargava, ML Klein
The Journal of Physical Chemistry A 113 (10), 1898-1904
- The effect of proton disorder on the structure of ice-Ih: A theoretical study** 65 2005
JL Kuo, ML Klein, WF Kuhs
The Journal of chemical physics 123 (13), 134505
- Structure and dynamics of associated molecular systems. III. Computer simulation of liquid hydrogen chloride** 65 1980
IR McDonald, SF O'Shea, DG Bounds, ML Klein
The Journal of Chemical Physics 72 (10), 5710-5717
- Raft registration across bilayers in a molecularly detailed model** 64 2011
DA Pantano, PB Moore, ML Klein, DE Discher
Soft Matter 7 (18), 8182-8191
- First principles effective electronic couplings for hole transfer in natural and size-expanded DNA** 64 2009
A Migliore, S Corni, D Varsano, ML Klein, R Di Felice
The Journal of Physical Chemistry B 113 (28), 9402-9415
- Proton shuttles and phosphatase activity in soluble epoxide hydrolase** 64 2007
M De Vivo, B Ensing, M Dal Peraro, GA Gomez, DW Christianson, ...
Journal of the American Chemical Society 129 (2), 387-394
- Transmembrane peptide-induced lipid sorting and mechanism of L α -to-inverted phase transition using coarse-grain molecular dynamics** 64 2004
SO Nielsen, CF Lopez, I Ivanov, PB Moore, JC Shelley, ML Klein
Biophysical journal 87 (4), 2107-2115
- Molecular dynamics investigation of membrane-bound bundles of the channel-forming transmembrane domain of viral protein U from the human immunodeficiency virus HIV-1** 64 2002
CF Lopez, M Montal, JK Blasie, ML Klein, PB Moore
Biophysical journal 83 (3), 1259-1267

- Nature of lithium trapping sites in the quantum solids *para*-hydrogen and *ortho*-deuterium** 64 1993
D Scharf, GJ Martyna, D Li, GA Voth, ML Klein
The Journal of chemical physics 99 (11), 9013-9020
- Computer simulation of a quantum particle in a quenched disordered system: Direct observation of Lifshitz traps** 64 1985
M Sprik, ML Klein, D Chandler
Physical Review B 32 (1), 545
- Gating pore currents are defects in common with two Na_v1.5 mutations in patients with mixed arrhythmias and dilated cardiomyopathy** 63 2015
A Moreau, P Gosselin-Badaroudine, L Delemotte, ML Klein, M Chahine
Journal of General Physiology 145 (2), 93-106
- Coarse-grained force field for ionic surfactants** 63 2011
W Shinoda, R DeVane, ML Klein
Soft Matter 7 (13), 6178-6186
- Gemini surfactants at the air/water interface: a fully atomistic molecular dynamics study** 63 2006
E Khurana, SO Nielsen, ML Klein
The Journal of Physical Chemistry B 110 (44), 22136-22142
- Evolutionary imprint of activation: The design principles of VSDs** 62 2014
E Palovcak, L Delemotte, ML Klein, V Carnevale
Journal of General Physiology 143 (2), 145-156
- Sodium ion binding sites and hydration in the lumen of a bacterial ion channel from molecular dynamics simulations** 62 2011
V Carnevale, W Treptow, ML Klein
The Journal of Physical Chemistry Letters 2 (19), 2504-2508
- Exploring the gating mechanism in the ClC chloride channel via metadynamics** 62 2006
FL Gervasio, M Parrinello, M Ceccarelli, ML Klein
Journal of molecular biology 361 (2), 390-398
- Relative pK_a Values from First-Principles Molecular Dynamics: The Case of Histidine Deprotonation** 62 2006
I Ivanov, B Chen, S Raugei, ML Klein
The Journal of Physical Chemistry B 110 (12), 6365-6371
- Toward a statistical thermodynamics of steady states** 62 1997
ME Tuckerman, CJ Mundy, ML Klein
Physical review letters 78 (11), 2042
- Lattice vibrations of ices Ih, VIII, and IX** 62 1984

- JS Tse, ML Klein, IR McDonald
The Journal of chemical physics 81 (12), 6124-6129
- [New High-Pressure Phase of Solid He 4 Is bcc](#) 62 1983
D Lévesque, JJ Weis, ML Klein
Physical Review Letters 51 (8), 670
- [Phonon Energies and Lifetimes in Solid Ne and He in the First-Order Self-Consistent Approximation](#) 62 1970
VV Goldman, GK Horton, ML Klein
Physical Review Letters 24 (25), 1424
- [Modulation of a voltage-gated Na⁺ channel by sevoflurane involves multiple sites and distinct mechanisms](#) 61 2014
AF Barber, V Carnevale, ML Klein, RG Eckenhoff, M Covarrubias
Proceedings of the National Academy of Sciences 111 (18), 6726-6731
- [Exploring conformational states of the bacterial voltage-gated sodium channel NavAb via molecular dynamics simulations](#) 61 2012
C Amaral, V Carnevale, ML Klein, W Treptow
Proceedings of the National Academy of Sciences 109 (52), 21336-21341
- [Atomistic simulation study of linear alkylbenzene sulfonates at the water/air interface](#) 61 2010
X He, O Guvench, AD MacKerell Jr, ML Klein
The Journal of Physical Chemistry B 114 (30), 9787-9794
- [Coarse-grained potential models for phenyl-based molecules: I. Parametrization using experimental data](#) 61 2010
R DeVane, ML Klein, C Chiu, SO Nielsen, W Shinoda, PB Moore
The Journal of Physical Chemistry B 114 (19), 6386-6393
- [Simulating the nucleation of water/ethanol and water/n-nonane mixtures: Mutual enhancement and two-pathway mechanism](#) 61 2003
B Chen, JI Siepmann, ML Klein
Journal of the American Chemical Society 125 (10), 3113-3118
- [Short wavelength collective dynamics in phospholipid bilayers: a molecular dynamics study](#) 61 2001
M Tarek, DJ Tobias, SH Chen, ML Klein
Physical Review Letters 87 (23), 238101
- [Molecular dynamics simulations of supported phospholipid/alkanethiol bilayers on a gold \(111\) surface](#) 61 1999
M Tarek, K Tu, ML Klein, DJ Tobias
Biophysical journal 77 (2), 964-972
- [Molecular dynamics investigation of a newtonian black film](#) 61 1992
Z Gamba, J Hautman, JC Shelley, ML Klein
Langmuir 8 (12), 3155-3160

- Elastic response of a simple amorphous binary alloy near the glass transition** 61 1988
 JL Barrat, JN Roux, JP Hansen, ML Klein
 EPL (Europhysics Letters) 7 (8), 707
- Elastic constants of solid Ar, Kr, and Xe: a Monte Carlo study** 61 1972
 ML Klein, RD Murphy
 Physical Review B 6 (6), 2433
- Frustrated solvation structures can enhance electron transfer rates** 60 2015
 RC Remsing, IG McKendry, DR Strongin, ML Klein, MJ Zdilla
 The journal of physical chemistry letters 6 (23), 4804-4808
- Supramolecular polymerization of benzene-1, 3, 5-tricarboxamide: a molecular dynamics simulation study** 60 2014
 KK Bejagam, G Fiorin, ML Klein, S Balasubramanian
 The Journal of Physical Chemistry B 118 (19), 5218-5228
- Structure and dynamics of bipolarons in liquid ammonia** 60 1992
 Z Deng, GJ Martyna, ML Klein
 Physical review letters 68 (16), 2496
- Monte Carlo calculations for solid and liquid argon** 60 1973
 JA Barker, ML Klein
 Physical Review B 7 (10), 4707
- Free-energy landscape of ion-channel voltage-sensor-domain activation** 58 2015
 L Delemotte, MA Kasimova, ML Klein, M Tarek, V Carnevale
 Proceedings of the National Academy of Sciences 112 (1), 124-129
- Conduction in a biological sodium selective channel** 58 2013
 L Stock, L Delemotte, V Carnevale, W Treptow, ML Klein
 The journal of physical chemistry B 117 (14), 3782-3789
- Inert gases: potentials, dynamics, and energy transfer in doped crystals** 58 * 2012
 RA Aziz, SS Cohen, H Dubost
 Springer Science & Business Media
- Polyethylene under tensile load: Strain energy storage and breaking of linear and knotted alkanes probed by first-principles molecular dynamics calculations** 58 1999
 AM Saitta, ML Klein
 The Journal of chemical physics 111 (20), 9434-9440
- Molecular dynamics simulations of a protein on hydrophobic and hydrophilic surfaces** 58 1996
 DJ Tobias, W Mar, JK Blasie, ML Klein
 Biophysical Journal 71 (6), 2933-2941

- Lattice vibrations and infrared absorption of ice Ih** 58 1986
M Marchi, JS Tse, ML Klein
The Journal of chemical physics 85 (5), 2414-2418
- Coarse-grained molecular dynamics study of membrane fusion: Curvature effects on free energy barriers along the stalk mechanism** 57 2015
S Kawamoto, ML Klein, W Shinoda
The Journal of Chemical Physics 143 (24), 243112
- Effect of sensor domain mutations on the properties of voltage-gated ion channels: molecular dynamics studies of the potassium channel Kv1. 2** 57 2010
L Delemotte, W Treptow, ML Klein, M Tarek
Biophysical Journal 99 (9), L72-L74
- Understanding the effect of magnesium ion concentration on the catalytic activity of ribonuclease H through computation: does a third metal binding site modulate endonuclease ...** 57 2010
MH Ho, M De Vivo, M Dal Peraro, ML Klein
Journal of the American Chemical Society 132 (39), 13702-13712
- Exploring the utility of coarse-grained water models for computational studies of interfacial systems** 57 2010
X He, W Shinoda, R DeVane, ML Klein
Molecular Physics 108 (15), 2007-2020
- Modeling the charge distribution at metal sites in proteins for molecular dynamics simulations** 57 2007
M Dal Peraro, K Spiegel, G Lamoureux, M De Vivo, WF DeGrado, ...
Journal of structural biology 157 (3), 444-453
- Dynamical behavior of the azide ion in protic solvents** 57 1993
M Ferrario, ML Klein, IR McDonald
Chemical physics letters 213 (5-6), 537-540
- The dynamical structure factor $S(Q, \omega)$ of solid β -N₂** 57 1977
ML Klein, JJ Weis
The Journal of Chemical Physics 67 (1), 217-224
- Nanoscale carbon particles and the stability of lipid bilayers** 56 2011
A Jusufi, RH DeVane, W Shinoda, ML Klein
Soft Matter 7 (3), 1139-1146
- Molecular dynamics study of the effect of surfactant on a biomembrane** 56 2001
S Bandyopadhyay, JC Shelley, ML Klein
The Journal of Physical Chemistry B 105 (25), 5979-5986
- Thermal and elastic properties of crystals at low temperatures** 56 1962
THK Barron, ML Klein
Physical Review 127 (6), 1997

- Exploring functional pairing between surface glycoconjugates and human galectins using programmable glycodendrimersomes** 55 2018
Q Xiao, AK Ludwig, C Romanò, I Buzzacchera, SE Sherman, M Vetro, ...
Proceedings of the National Academy of Sciences 115 (11), E2509-E2518
- Aqueous solutions of imidazolium ionic liquids: molecular dynamics studies** 55 2009
BL Bhargava, ML Klein
Soft Matter 5 (18), 3475-3480
- Quantum simulation studies of singlet and triplet bipolarons in liquid ammonia** 55 1993
GJ Martyna, Z Deng, ML Klein
The Journal of chemical physics 98 (1), 555-563
- Molecular dynamics simulation of the plastic phase of solid methane** 55 1980
DG Bounds, ML Klein, GN Patey
The Journal of Chemical Physics 72 (10), 5348-5356
- Comparative sequence analysis suggests a conserved gating mechanism for TRP channels** 54 2015
E Palovcak, L Delemotte, ML Klein, V Carnevale
Journal of General Physiology 146 (1), 37-50
- Identification of a fluorescent general anesthetic, 1-aminoanthracene** 54 2009
CA Butts, J Xi, G Brannigan, AA Saad, SP Venkatachalan, RA Pearce, ...
Proceedings of the National Academy of Sciences 106 (16), 6501-6506
- Molecular dynamics investigation of an ethanol-water solution** 54 1996
M Tarek, DJ Tobias, ML Klein
Physica A: Statistical Mechanics and its Applications 231 (1-3), 117-122
- Molecular dynamics studies of sodium octanoate and water: the liquid-crystal mesophase with two-dimensional hexagonal symmetry** 54 1991
K Watanabe, ML Klein
The Journal of Physical Chemistry 95 (10), 4158-4166
- Janus dendrimersomes coassembled from fluorinated, hydrogenated, and hybrid Janus dendrimers as models for cell fusion and fission** 53 2017
Q Xiao, SE Sherman, SE Wilner, X Zhou, C Dazen, T Baumgart, EH Reed, ...
Proceedings of the National Academy of Sciences 114 (34), E7045-E7053
- Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes** 53 2015
CM MacDermaid, HK Kashyap, RH DeVane, W Shinoda, JB Klauda, ...
The Journal of chemical physics 143 (24), 12B625_1
- Initial response of the potassium channel voltage sensor to a transmembrane potential** 53 2009
W Treptow, M Tarek, ML Klein

Journal of the American Chemical Society 131 (6), 2107-2109

[Self-assembling cyclic peptides: molecular dynamics studies of dimers in polar and nonpolar solvents](#) 53 2006

E Khurana, SO Nielsen, B Ensing, ML Klein
The Journal of Physical Chemistry B 110 (38), 18965-18972

[Structural and spectral properties of aqueous hydrogen fluoride studied using ab initio molecular dynamics](#) 53 2002

AJ Sillanpää, C Simon, ML Klein, K Laasonen
The Journal of Physical Chemistry B 106 (43), 11315-11322

[Self-assembly of a phospholipid Langmuir monolayer using coarse-grained molecular dynamics simulations](#) 53 2002

CF Lopez, SO Nielsen, PB Moore, JC Shelley, ML Klein
Journal of Physics: Condensed Matter 14 (40), 9431

[Intermolecular potentials and the properties of liquid and solid hydrogen sulphide](#) 53 1989

TR Forester, IR McDonald, ML Klein
Chemical physics 129 (2), 225-234

[Structural and dynamic properties of lithium sulphate in its solid electrolyte form](#) 53 1985

RW Impey, ML Klein, IR McDonald
The Journal of chemical physics 82 (10), 4690-4698

[Orientational order in ionic crystals containing tetrahedral ions](#) 53 1983

ML Klein, IR McDonald, Y Ozaki
The Journal of chemical physics 79 (11), 5579-5587

[Design–functionality relationships for adhesion/growth-regulatory galectins](#) 51 2019

AK Ludwig, M Michalak, Q Xiao, U Gilles, FJ Medrano, H Ma, ...
Proceedings of the National Academy of Sciences 116 (8), 2837-2842

[Initial stages of aggregation in aqueous solutions of ionic liquids: molecular dynamics studies](#) 51 2009

BL Bhargava, ML Klein
The Journal of Physical Chemistry B 113 (28), 9499-9505

[Structural and dynamical behavior of an azide anion in water from ab initio molecular dynamics calculations](#) 51 2000

DA Yarne, ME Tuckerman, ML Klein
Chemical Physics 258 (2-3), 163-169

[Premicelles and monomer exchange in aqueous surfactant solutions above and below the critical micelle concentration](#) 50 2012

DN LeBard, BG Levine, R DeVane, W Shinoda, ML Klein
Chemical Physics Letters 522, 38-42

- Structure of Ice-VII and Ice-VIII: A quantum mechanical study** 50 2004
JL Kuo, ML Klein
The Journal of Physical Chemistry B 108 (51), 19634-19639
- Influence of anesthetic and nonimmobilizer molecules on the physical properties of a polyunsaturated lipid bilayer** 50 2003
L Koubi, L Saiz, M Tarek, D Scharf, ML Klein
The Journal of Physical Chemistry B 107 (51), 14500-14508
- Molecular dynamics studies of aqueous surfactants systems** 50 1998
M Tarek, S Bandyopadhyay, ML Klein
Journal of molecular liquids 78 (1-2), 1-6
- Quantum simulation studies of metal-ammonia solutions** 50 1994
Z Deng, GJ Martyna, ML Klein
The Journal of chemical physics 100 (10), 7590-7601
- Isotopic shift in the melting curve of helium: A path integral Monte Carlo study** 50 1989
JL Barrat, P Loubeyre, ML Klein
The Journal of chemical physics 90 (10), 5644-5650
- Optimization of a distributed Gaussian basis set using simulated annealing: Application to the solvated electron** 50 1987
M Sprik, ML Klein
The Journal of chemical physics 87 (10), 5987-5999
- Analysis of translation-rotation coupling in an orientationally disordered ionic crystal** 50 1983
RM Lynden-Bell, IR McDonald, ML Klein
Molecular Physics 48 (5), 1093-1117
- Structure and dynamics of associated molecular systems. II. Atom-atom potentials and the properties of ammonia** 50 1979
ML Klein, IR McDonald, R Righini
The Journal of Chemical Physics 71 (9), 3673-3682
- Formation of micelles in aqueous solutions of a room temperature ionic liquid: a study using coarse grained molecular dynamics** 49 2009
BL Bhargava, M L. Klein
Molecular Physics 107 (4-6), 393-401
- A stable water chain in the hydrophobic pore of the AmtB ammonium transporter** 49 2007
G Lamoureux, ML Klein, S Bernèche
Biophysical journal 92 (9), L82-L84
- Structure of solid poly (tetrafluoroethylene): A computer simulation study of chain orientational, translational, and conformational disorder** 49 1997

- M Sprik, U Röthlisberger, ML Klein
The Journal of Physical Chemistry B 101 (15), 2745-2749
- Electronic states and dynamical behavior of LiXe_n and CsXe_n clusters** 49 1991
G Martyna, C Cheng, ML Klein
The Journal of chemical physics 95 (2), 1318-1336
- Pseudopotential calculation of the electronic states of small metal-ammonia clusters** 49 1991
GJ Martyna, ML Klein
The Journal of Physical Chemistry 95 (2), 515-518
- Study of electron solvation in polar solvents using path integral calculations** 49 1986
M Sprik, RW Impey, ML Klein
Journal of Statistical Physics 43 (5/6), 967-972
- Molecular-dynamics study of solid $\gamma\text{-O}_2$** 49 1980
ML Klein, D Levesque, JJ Weis
Physical Review B 21 (12), 5785
- Solution NMR structure of a designed metalloprotein and complementary molecular dynamics refinement** 48 2008
JR Calhoun, W Liu, K Spiegel, M Dal Peraro, ML Klein, KG Valentine, ...
Structure 16 (2), 210-215
- Computational study of phosphatase activity in soluble epoxide hydrolase: high efficiency through a water bridge mediated proton shuttle** 48 2005
M De Vivo, B Ensing, ML Klein
Journal of the American Chemical Society 127 (32), 11226-11227
- Assessment of all-atom potentials for modeling membranes: molecular dynamics simulations of solid and liquid alkanes and crystals of phospholipid fragments** 48 1997
DJ Tobias, K Tu, ML Klein
Journal de chimie physique 94, 1482-1502
- Isotope effect on the melting of para-hydrogen and ortho-deuterium clusters** 48 1992
D Scharf, GJ Martyna, ML Klein
Chemical physics letters 197 (3), 231-235
- Dynamic properties of the structure II clathrate hydrate of krypton** 48 1987
JS Tse, ML Klein
Journal of Physical Chemistry 91 (22), 5789-5791
- Lattice dynamics in solid oxygen** 48 1979
K Kobashi, ML Klein, V Chandrasekharan
The Journal of Chemical Physics 71 (2), 843-849
- Intermolecular interactions and the structure of fatty acid- soap crystals** 47 2001
ML Lynch, F Wireko, M Tarek, M Klein

The Journal of Physical Chemistry B 105 (2), 552-561

- [Two possible conducting states of the influenza A virus M2 ion channel](#) 47 2000
Q Zhong, DM Newns, P Pattnaik, JD Lear, ML Klein
FEBS letters 473 (2), 195-198
- [Computer simulations and the interpretation of incoherent neutron scattering experiments on the solid rotator phases of long-chain alkanes](#) 47 1994
JP Ryckaert, ML Klein, IR McDonald
Molecular Physics 83 (3), 439-458
- [Coarse-grained potential models for phenyl-based molecules: II. Application to fullerenes](#) 46 2010
C Chiu, R DeVane, ML Klein, W Shinoda, PB Moore, SO Nielsen
The Journal of Physical Chemistry B 114 (19), 6394-6400
- [Controlling the shape and flexibility of arylamides: a combined ab initio, ab initio molecular dynamics, and classical molecular dynamics study](#) 46 2006
V Pophristic, S Vemparala, I Ivanov, Z Liu, ML Klein, WF DeGrado
The Journal of Physical Chemistry B 110 (8), 3517-3526
- [Role of aromatic localization in the gating process of a potassium channel](#) 46 2006
C Domene, S Vemparala, ML Klein, C Vénien-Bryan, DA Doyle
Biophysical journal 90 (1), L01-L03
- [Characterization of the dizinc analogue of the synthetic diiron protein DF1 using ab initio and hybrid quantum/classical molecular dynamics simulations](#) 46 2003
A Magistrato, WF DeGrado, A Laio, U Rothlisberger, J VandeVondele, ...
The Journal of Physical Chemistry B 107 (17), 4182-4188
- [Ab initio molecular dynamics investigation of singlet C2H2Li2: determination of the ground state structure and observation of LiH intermediates](#) 46 1995
U Rothlisberger, ML Klein
Journal of the American Chemical Society 117 (1), 42-48
- [Structure and energetics of fluid para-hydrogen](#) 46 1993
D Scharf, GJ Martyna, ML Klein
Fizika Nizkikh Temperatur 19 (5), 516-519
- [Solvation and ionisation of alkali metals in liquid ammonia: a path integral Monte Carlo study](#) 46 1990
M Marchi, M Sprik, ML Klein
Journal of Physics: Condensed Matter 2 (26), 5833
- [Adiabatic dynamics of the solvated electron in liquid ammonia](#) 46 1989
M Sprik, ML Klein
The Journal of chemical physics 91 (9), 5665-5671
- [Anisotropy of the Electrostatic Interactions and the Properties of](#) 46 1981

Orientationally Disordered Cyanide Crystals

DG Bounds, ML Klein, IR McDonald
Physical Review Letters 46 (26), 1682

An intermolecular potential for (NH₃)₂

G Duquette, TH Ellis, G Scoles, RO Watts, ML Klein
The Journal of Chemical Physics 68 (6), 2544-2549

Anharmonic effects in the phonon spectra of sodium chloride

ER Cowley, G Jacucci, ML Klein, IR McDonald
Physical Review B 14 (4), 1758

Lattice Dynamics with Three-Body Forces. II. Krypton

MV Bobetic, JA Barker, ML Klein
Physical Review B 5 (8), 3185

A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory

A Bankura, B Santra, RA DiStasio Jr, CW Swartz, ML Klein, X Wu
Molecular Physics 113 (17-18), 2842-2854

Formation of interconnected aggregates in aqueous dicationic ionic liquid solutions

BL Bhargava, ML Klein
Journal of Chemical Theory and Computation 6 (3), 873-879

Parameterization of azole-bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure

K Spiegel, A Magistrato, P Maurer, P Ruggerone, U Rothlisberger, ...
Journal of computational chemistry 29 (1), 38-49

Computer simulation of aqueous block copolymer assemblies: length scales and methods

V Ortiz, SO Nielsen, ML Klein, DE Discher
Journal of Polymer Science Part B: Polymer Physics 44 (14), 1907-1918

Conformational and orientational order and disorder in solid polytetrafluoroethylene

M Sprik, U Rothlisberger, ML Klein
Molecular Physics 97 (3), 355-373

Economic integration between Hong Kong, Taiwan and the coastal provinces of China

RS Jones, RE King, M Klein
OECD Economic Studies, 115-115

Anion ordering in alkali cyanide crystals

M Ferrario, IR McDonald, ML Klein
The Journal of chemical physics 84 (7), 3975-3985

46 1978

46 1976

46 1972

45 2015

45 2010

45 2008

45 2006

45 1999

45 1993

45 1986

- Properties of solid potassium cyanide: Is the physics of cyanide crystals really chemistry?** 45 1983
ML Klein, IR McDonald
The Journal of chemical physics 79 (5), 2333-2342
- The role of conformation in ion permeation in a K⁺ channel** 44 2008
C Domene, S Vemparala, S Furini, K Sharp, ML Klein
Journal of the American Chemical Society 130 (11), 3389-3398
- Random Strains and the Structure of (KBr)_{1-x}(KCN)_x Mixed Crystals** 44 1986
LJ Lewis, ML Klein
Physical review letters 57 (21), 2698
- TCR triggering by pMHC ligands tethered on surfaces via poly (ethylene glycol) depends on polymer length** 43 2014
Z Ma, DN LeBard, SM Loverde, KA Sharp, ML Klein, DE Discher, ...
PloS one 9 (11), e112292
- Facially amphiphilic polymers as anti-infective agents** 43 * 2007
WF Degrado, GN Tew, ML Klein, D Liu, J Yuan
US Patent 7,173,102
- Molecular dynamics study of the LS3 voltage-gated ion channel** 43 1998
Q Zhong, PB Moore, DM News, ML Klein
FEBS letters 427 (2), 267-270
- Ab initio molecular dynamics study of solid nitromethane** 43 1998
ME Tuckerman, ML Klein
Chemical physics letters 283 (3-4), 147-151
- Is hydrogen chloride an associated liquid?** 43 1981
ML Klein, IR McDonald
Molecular Physics 42 (1), 243-247
- Radial distribution function of liquid sodium** 43 1973
RD Murphy, ML Klein
Physical Review A 8 (5), 2640
- Computational study of drug binding to the membrane-bound tetrameric M2 peptide bundle from influenza A virus** 42 2011
E Khurana, RH DeVane, M Dal Peraro, ML Klein
Biochimica et Biophysica Acta (BBA)-Biomembranes 1808 (2), 530-537
- Evaluation of Electronic Coupling in Transition-Metal Systems Using DFT: Application to the Hexa-Aquo Ferric- Ferrous Redox Couple** 42 2009
A Migliore, PHL Sit, ML Klein
Journal of Chemical Theory and Computation 5 (2), 307-323
- Structural Correlations and Charge Ordering in a Room-Temperature Ionic** 42 2008

Liquid

BL Bhargava, ML Klein, S Balasubramanian
ChemPhysChem 9 (1), 67-70

Modeling surfactant adsorption on hydrophobic surfaces 42 2005

SO Nielsen, G Srinivas, CF Lopez, ML Klein
Physical review letters 94 (22), 228301

Molecular dynamics simulations of a hydrated protein vectorially oriented on polar and nonpolar soft surfaces 42 2002

CE Nordgren, DJ Tobias, ML Klein, JK Blasie
Biophysical journal 83 (6), 2906-2917

Infrared spectrum of two fullerene derivatives: C60O and C61H2 42 1994

G Cardini, R Bini, PR Salvi, V Schettino, ML Klein, RM Strongin, L Brard, ...
The Journal of Physical Chemistry 98 (40), 9966-9971

Intermolecular potentials and the simulation of liquid water 42 1978

IR McDonald, ML Klein
The Journal of Chemical Physics 68 (11), 4875-4877

Lattice Dynamics of fcc Argon with Three-Body Forces 42 1971

ML Klein, JA Barker, TR Koehler
Physical Review B 4 (6), 1983

Thermodynamic properties of solid Ar, Kr and Xe based upon a short range central force and the improved self-consistent phonon scheme 42 1970

ML Klein, VV Goldman, GK Horton
Journal of Physics and Chemistry of Solids 31 (11), 2441-2452

Ab initio molecular dynamics study of polyfluoride anions 41 1997

T von Roseninge, M Parrinello, ML Klein
The Journal of chemical physics 107 (19), 8012-8019

Structure of CaI_{12} 41 1995

AP Seitsonen, K Laasonen, RM Nieminen, ML Klein
The Journal of chemical physics 103 (18), 8075-8080

Lattice dynamics of Rb 71 K 29: Molecular dynamics study 41 1978

G Jacucci, ML Klein, R Taylor
Physical Review B 18 (8), 3782

Science 1997, 275, 817 41

ME Tuckerman, D Marx, ML Klein, M Parrinello
Google Scholar There is no corresponding record for this reference

Nuclear quantum effects on the structure and energetics of $(H_2O)_6 H^+$ 40 2005

M Mella, JL Kuo, DC Clary, ML Klein
Physical Chemistry Chemical Physics 7 (11), 2324-2332

- Water on the Move** 40 2001
ML Klein
Science 291 (5511), 2106-2107
- A molecular dynamics study of the low temperature structure and dynamics of ethane monolayers physisorbed on the graphite basal plane** 40 1989
MA Moller, ML Klein
The Journal of chemical physics 90 (3), 1960-1967
- Hydration structure of Na⁺ and K⁺ from ab initio molecular dynamics based on modern density functional theory** 39 2014
A Bankura, V Carnevale, ML Klein
Molecular Physics 112 (9-10), 1448-1456
- Delivery quality assurance with ArcCHECK** 39 2013
C Neilson, M Klein, R Barnett, S Yartsev
Medical Dosimetry 38 (1), 77-80
- Curvature, rigidity, and pattern formation in functional polymer micelles and vesicles—From dynamic visualization to molecular simulation** 39 2011
SM Loverde, DA Pantano, DA Christian, A Mahmud, ML Klein, DE Discher
Current Opinion in Solid State and Materials Science 15 (6), 277-284
- Probing peptide nanotube self-assembly at a liquid– liquid interface with coarse-grained molecular dynamics** 39 2008
E Khurana, RH DeVane, A Kohlmeyer, ML Klein
Nano letters 8 (11), 3626-3630
- Azole-bridged diplatinum anticancer compounds. Modulating DNA flexibility to escape repair mechanism and avoid cross resistance** 39 2007
K Spiegel, A Magistrato, P Carloni, J Reedijk, ML Klein
The Journal of Physical Chemistry B 111 (41), 11873-11876
- Dissociation of hydrogen fluoride in HF(H₂O)₇** 39 2004
JL Kuo, ML Klein
The Journal of chemical physics 120 (10), 4690-4695
- Acyl chain conformation and packing in dipalmitoylphosphatidylcholine bilayers from MD simulation and IR spectroscopy** 39 2002
RG Snyder, K Tu, ML Klein, R Mendelssohn, HL Strauss, W Sun
The Journal of Physical Chemistry B 106 (24), 6273-6288
- Centroid path integral molecular-dynamics studies of a para-hydrogen slab containing a lithium impurity** 39 1998
K Kinugawa, PB Moore, ML Klein
The Journal of chemical physics 109 (2), 610-617
- Solvation of electrons, atoms and ions in liquid ammonia** 39 1988
M Marchi, M Sprik, ML Klein

Faraday Discussions of the Chemical Society 85, 373-389

Ground-state properties of xenon on graphite

39 1983

B Joos, B Bergersen, ML Klein
Physical Review B 28 (12), 7219

Encoding biological recognition in a bicomponent cell-membrane mimic

38 2019

C Rodriguez-Emmenegger, Q Xiao, NY Kostina, SE Sherman, K Rahimi, ...
Proceedings of the National Academy of Sciences 116 (12), 5376-5382

Nanoscale organization in aqueous dicationic ionic liquid solutions

38 2011

BL Bhargava, ML Klein
The Journal of Physical Chemistry B 115 (35), 10439-10446

Computational studies on the interactions of inhalational anesthetics with proteins

38 2010

S Vemparala, C Domene, ML Klein
Accounts of chemical research 43 (1), 103-110

Controlling the conformation of arylamides: computational studies of intramolecular hydrogen bonds between amides and ethers or thioethers

38 2004

RJ Doerksen, B Chen, D Liu, GN Tew, WF DeGrado, ML Klein
Chemistry—A European Journal 10 (20), 5008-5016

Coarse-grain molecular dynamics simulations of diblock copolymer surfactants interacting with a lipid bilayer

38 2004

G Srinivas*, ML Klein
Molecular Physics 102 (9-10), 883-889

Introductory lecture. Conformations of flexible molecules in fluid phases

38 1992

ML Klein
Journal of the Chemical Society, Faraday Transactions 88 (13), 1701-1705

Pressure induced amorphization of ice I_h

38 1990

JS Tse, ML Klein
The Journal of chemical physics 92 (6), 3992-3994

A theoretical study of the lattice dynamics of neon and its isotopes

38 1969

VV Goldman, GK Horton, ML Klein
Journal of Low Temperature Physics 1 (5), 391-405

Reaction of a programmable glycan presentation of glycodendrimersomes and cells with engineered human lectins to show the sugar functionality of the cell surface

37 2017

J Kopitz, Q Xiao, AK Ludwig, A Romero, M Michalak, SE Sherman, X Zhou, ...
Angewandte Chemie International Edition 56 (46), 14677-14681

Hinge-bending motions in the pore domain of a bacterial voltage-gated sodium channel

37 2012

AF Barber, V Carnevale, SG Raju, C Amaral, W Treptow, ML Klein

Biochimica et Biophysica Acta (BBA)-Biomembranes 1818 (9), 2120-2125

- Surfactant concentration effects on micellar properties** 37 2012
 A Jusufi, DN LeBard, BG Levine, ML Klein
 The Journal of Physical Chemistry B 116 (3), 987-991
- Influence of highly polyunsaturated lipid acyl chains of biomembranes on the NMR order parameters** 37 2001
 L Saiz, ML Klein
 Journal of the American Chemical Society 123 (30), 7381-7387
- Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations** 37 1988
 M Marchi, M Sprik, ML Klein
 The Journal of chemical physics 89 (8), 4918-4923
- Orientalional phases of classical octopoles on a triangular lattice and the adsorption of methane on graphite** 37 1979
 SF O'Shea, ML Klein
 The Journal of Chemical Physics 71 (6), 2399-2403
- Electron-hole theory of the effect of quantum nuclei on the X-ray absorption spectra of liquid water** 36 2018
 Z Sun, L Zheng, M Chen, ML Klein, F Paesani, X Wu
 Physical Review Letters 121 (13), 137401
- Implicit-solvent models for micellization: nonionic surfactants and temperature-dependent properties** 36 2011
 A Jusufi, S Sanders, ML Klein, AZ Panagiotopoulos
 The Journal of Physical Chemistry B 115 (5), 990-1001
- Parametrization and application of a coarse grained force field for benzene/fullerene interactions with lipids** 36 2010
 R DeVane, A Jusufi, W Shinoda, C Chiu, SO Nielsen, PB Moore, ML Klein
 The Journal of Physical Chemistry B 114 (49), 16364-16372
- Molecular dynamics study of two-component systems: The shape and surface structure of water/ethanol droplets** 36 1997
 M Tarek, ML Klein
 The Journal of Physical Chemistry A 101 (46), 8639-8642
- The Chinese economic area: economic integration without a free trade agreement** 36 1992
 RS Jones, R King, M Klein
 OECD
- A molecular dynamics study of the effect of pressure on the properties of water and ice** 36 1988
 JS Tse, ML Klein
 The Journal of Physical Chemistry 92 (2), 315-318

- [Constant-temperature–constant-pressure molecular-dynamics calculations for molecular solids: Application to solid nitrogen at high pressure](#) 36 1986
S Nosé, ML Klein
Physical Review B 33 (1), 339
- [Self-Consistent Theory of Second-Order Elastic Constants with an Application to Noble-Gas Crystals](#) 36 1970
ML Klein, GK Horton, VV Goldman
Physical Review B 2 (12), 4995
- [Bioactive cell-like hybrids from dendrimersomes with a human cell membrane and its components](#) 35 2019
SS Yadavalli, Q Xiao, SE Sherman, WD Hasley, ML Klein, M Goulian, ...
Proceedings of the National Academy of Sciences 116 (3), 744-752
- [Molecular dynamics simulations of voltage-gated cation channels: insights on voltage-sensor domain function and modulation](#) 35 2012
L Delemotte, ML Klein, M Tarek
Frontiers in Pharmacology 3, 97
- [Computer simulation studies of amphiphilic interfaces](#) 35 1998
S Bandyopadhyay, M Tarek, ML Klein
Current opinion in colloid & interface science 3 (3), 242-246
- [Solid C 70: A molecular-dynamics study of the structure and orientational ordering](#) 35 1992
A Cheng, ML Klein
Physical Review B 46 (8), 4958
- [Simulation of liquid ammonia](#) 35 1976
IR McDonald, ML Klein
The Journal of Chemical Physics 64 (11), 4790-4791
- [Multiple proton confinement in the M2 channel from the influenza A virus](#) 34 2010
V Carnevale, G Fiorin, BG Levine, WF DeGrado, ML Klein
The Journal of Physical Chemistry C 114 (48), 20856-20863
- [Unraveling the catalytic pathway of metalloenzyme farnesyltransferase through QM/MM computation](#) 34 2009
MH Ho, MD Vivo, MD Peraro, ML Klein
Journal of Chemical Theory and Computation 5 (6), 1657-1666
- [Revisiting the free energy profile for the nucleophilic attack of hydroxide on formamide in aqueous solution](#) 34 2006
J Blumberger, ML Klein
Chemical physics letters 422 (1-3), 210-217
- [First-principles molecular dynamics study of the rupture processes of a](#) 34 2001

- bulklike polyethylene knot**
AM Saitta, ML Klein
The Journal of Physical Chemistry B 105 (28), 6495-6499
- Constant pressure and temperature molecular dynamics simulations of crystals of the lecithin fragments: glycerylphosphorylcholine and dilauroylglycerol** 34 1995
K Tu, DJ Tobias, ML Klein
The Journal of Physical Chemistry 99 (24), 10035-10042
- The electronic states of lithium atoms in ammonia clusters and solution** 34 1992
GJ Martyna, ML Klein
The Journal of chemical physics 96 (10), 7662-7671
- Critical Fluctuations in the Paraelectric Phase of NaNO₂** 34 1982
ML Klein, IR McDonald, Y Ozaki
Physical Review Letters 48 (17), 1197
- The dynamical structure factor $S(Q, \omega)$ of solid α -N₂** 34 1975
JJ Weis, ML Klein
The Journal of Chemical Physics 63 (7), 2869-2873
- On the dissociation energy and interaction potential of ground-state Ne₂** 34 1974
RJ Le Roy, ML Klein, IJ McGee
Molecular Physics 28 (2), 587-591
- Ion channel sensing: Are fluctuations the crux of the matter?** 33 2018
MA Kasimova, A Yazici, Y Yudin, D Granata, ML Klein, T Rohacs, ...
The journal of physical chemistry letters 9 (6), 1260-1264
- Fluorine-19 NMR and computational quantification of isoflurane binding to the voltage-gated sodium channel NaChBac** 33 2016
MN Kinde, V Bondarenko, D Granata, W Bu, KC Grasty, PJ Loll, ...
Proceedings of the National Academy of Sciences 113 (48), 13762-13767
- Isolation of Acacetin from *Calea urticifolia* with Inhibitory Properties against Human Monoamine Oxidase-A and -B** 33 2016
ND Chaurasiya, V Gogineni, KM Elokely, F León, MJ Núñez, ML Klein, ...
Journal of Natural Products 79 (10), 2538-2544
- Methods, systems, and computer program products for computational analysis and design of amphiphilic polymers** 33 2009
R Doerksen, B Chen, WF Degrado, ML Klein
US Patent 7,590,517
- Models for phosphatidylglycerol lipids put to a structural test** 33 2009
J Hénin, W Shinoda, ML Klein
The Journal of Physical Chemistry B 113 (19), 6958-6963
- Modeling small aluminum chlorohydrate polymers** 33 2004

- V Pophristic, ML Klein, MN Holerca
The Journal of Physical Chemistry A 108 (1), 113-120
- [Structure and dynamics of the aluminum chlorohydrate polymer Al₁₃O₄\(OH\)₂₄\(H₂O\)₁₂Cl₇](#) 33 2004
V Pophristic, VSK Balagurusamy, ML Klein
Physical Chemistry Chemical Physics 6 (5), 919-923
- [Liquid hydrogen fluoride with an excess proton: ab initio molecular dynamics study of a superacid](#) 33 1999
D Kim, ML Klein
Journal of the American Chemical Society 121 (48), 11251-11252
- [Simulation studies of ultrathin films of linear and branched alkanes on a metal substrate](#) 33 1996
S Balasubramanian, ML Klein, JI Siepmann
The Journal of Physical Chemistry 100 (29), 11960-11963
- [Monte Carlo simulation of the liquid-vapor coexistence in a Langmuir monolayer of pentadecanoic acid](#) 33 1994
JI Siepmann, S Karaborni, ML Klein
The Journal of Physical Chemistry 98 (27), 6675-6678
- [Why do membranes of some unhealthy cells adopt a cubic architecture?](#) 32 2016
Q Xiao, Z Wang, D Williams, P Leowanawat, M Peterca, SE Sherman, ...
ACS central science 2 (12), 943-953
- [Asp44 stabilizes the Trp41 gate of the M2 proton channel of influenza A virus](#) 32 2013
C Ma, G Fiorin, V Carnevale, J Wang, RA Lamb, ML Klein, Y Wu, LH Pinto, ...
Structure 21 (11), 2033-2041
- [Ab initio molecular dynamics study of supercritical carbon dioxide including dispersion corrections](#) 32 2009
S Balasubramanian, A Kohlmeyer, ML Klein
The Journal of chemical physics 131 (14), 144506
- [The adsorption of acetylene on a graphite surface](#) 32 1986
C Peters, JA Morrison, ML Klein
Surface science 165 (2-3), 355-374
- [Molecular-dynamics calculations for ethylene adsorbed on graphite](#) 32 1984
S Nosé, ML Klein
Physical review letters 53 (8), 818
- [Probing the structure of PEGylated-lipid assemblies by coarse-grained molecular dynamics](#) 31 2013
W Shinoda, DE Discher, ML Klein, SM Loverde
Soft Matter 9 (48), 11549-11556

- Computational study of a nanobiosensor: a single-walled carbon nanotube functionalized with the Coxsackie-adenovirus receptor** 31 2009
RR Johnson, BJ Rego, ATC Johnson, ML Klein
The Journal of Physical Chemistry B 113 (34), 11589-11593
- Interaction of anesthetics with open and closed conformations of a potassium channel studied via molecular dynamics and normal mode analysis** 31 2008
S Vemparala, C Domene, ML Klein
Biophysical journal 94 (11), 4260-4269
- Effects of the nonimmobilizer hexafluoroethane on the model membrane dimyristoylphosphatidylcholine** 31 2002
L Koubi, M Tarek, S Bandyopadhyay, ML Klein, D Scharf
The Journal of the American Society of Anesthesiologists 97 (4), 848-855
- Are hydrogen atoms solvated by water molecules?** 31 1983
JS Tse, ML Klein
The Journal of Physical Chemistry 87 (25), 5055-5057
- A computer simulation of thermodynamic properties of solid Na** 31 1976
SS Cohen, ML Klein, MS Duesbery, R Taylor
Journal of Physics F: Metal Physics 6 (3), 337
- Self-consistent phonon spectrum of hcp H₂ and D₂** 31 1970
ML Klein, TR Koehler
Journal of Physics C: Solid State Physics 3 (5), L102
- Dependence of the structure and dynamics of liquid silicon on the choice of density functional approximation** 30 2017
RC Remsing, ML Klein, J Sun
Physical Review B 96 (2), 024203
- Complex Arrangement of Orthogonal Nanoscale Columns *via* a Supramolecular Orientational Memory Effect** 30 2016
M Peterca, MR Imam, SD Hudson, BE Partridge, D Sahoo, PA Heiney, ...
ACS nano 10 (11), 10480-10488
- The Membrane-Bound State of K_{2P} Potassium Channels** 30 2010
W Treptow, ML Klein
Journal of the American Chemical Society 132 (23), 8145-8151
- Ab initio molecular dynamics study of the superacid system SbF₅/HF solution** 30 2000
D Kim, ML Klein
The Journal of Physical Chemistry B 104 (43), 10074-10079
- Nonequilibrium molecular dynamics** 30 2000
CJ Mundy, S Balasubramanian, K Bagchi, ME Tuckerman, GJ Martyna, ...

Reviews in Computational Chemistry, 291-397

[The performance of density functional methods for the description of weak interaction potentials. The torsional potential of butane](#) 30 1994

U Röthlisberger, ML Klein
Chemical physics letters 227 (4-5), 390-395

[Simulation of the cubic to orthorhombic phase transition in potassium cyanide](#) 30 1985

RW Impey, M Sprik, ML Klein
The Journal of chemical physics 83 (7), 3638-3644

[An interatomic potential for Ne₂ derived from solid state data](#) 30 1973

VV Goldman, ML Klein
Journal of Low Temperature Physics 12 (1), 101-103

[Lattice dynamics of solid Kr](#) 30 1971

JA Barker, MV Bobetic, ML Klein
Physics Letters A 34 (7), 415-416

[Forces between adsorbed atoms and the determination of surface areas of solids](#) 30 1964

JD Johnson, ML Klein
Transactions of the Faraday Society 60

[Polymorphic phase transitions in alkali cyanide crystals](#) 29 1983

RW Impey, S Nosé, ML Klein
Molecular Physics 50 (1), 243-246

[Anharmonic lattice dynamics of solid potassium](#) 29 1977

HR Glyde, JP Hansen, ML Klein
Physical Review B 16 (8), 3476

[The static structure factor of liquid Li](#) 29 1976

G Jacucci, ML Klein, R Taylor
Solid State Communications 19 (7), 657-659

[Calculation of the Temperature Dependence of the Second-Order Elastic Constants of fcc Ar, Kr, and Xe Using a Two-Body Short-Range Interatomic Potential](#) 29 1969

C Feldman, ML Klein, GK Horton
Physical Review 184 (3), 910

[On the Strain Dependence of the Vibrational Frequency Distributions of Simple Lattices](#) 29 1963

THK Barron, ML Klein
Proceedings of the Physical Society (1958-1967) 82 (2), 161

[Does Proton Conduction in the Voltage-Gated H⁺ Channel hHv1 Involve](#) 28 2017

Grotthuss-Like Hopping via Acidic Residues?

SC van Keulen, E Gianti, V Carnevale, ML Klein, U Rothlisberger, ...
The Journal of Physical Chemistry B 121 (15), 3340-3351

Facially amphiphilic polymers and oligomers and uses thereof

WF DeGrado, GN Tew, ML Klein, D Liu, J Yuan, S Choi
US Patent 9,241,917

28 2016

Hydrogen-bonded water molecules in the M2 channel of the influenza A virus guide the binding preferences of ammonium-based inhibitors

E Gianti, V Carnevale, WF DeGrado, ML Klein, G Fiorin
The Journal of Physical Chemistry B 119 (3), 1173-1183

28 2015

Computational approaches to nanobiotechnology: probing the interaction of synthetic molecules with phospholipid bilayers via a coarse grain model

G Srinivas, ML Klein
Nanotechnology 15 (9), 1289

28 2004

First-principles study of bond rupture of entangled polymer chains

AM Saitta, ML Klein
The Journal of Physical Chemistry B 104 (10), 2197-2200

28 2000

Living polymers ab initio molecular dynamics study of the initiation step in the polymerization of isoprene induced by ethyl lithium

U Röthlisberger, M Sprik, ML Klein
Journal of the Chemical Society, Faraday Transactions 94 (4), 501-508

28 1998

Cation transport in lithium sulphate based crystals

M Ferrario, ML Klein, IR McDonald
Molecular Physics 86 (4), 923-938

28 1995

Molecular dynamics simulations of the structure and ion diffusion in poly(ethylene oxide)

K Laasonen, ML Klein
Journal of the Chemical Society, Faraday Transactions 91 (16), 2633-2638

28 1995

Nature of the Conduction States in the Metallic Molecular Crystal Li(NH₃)₄

J Kohanoff, F Buda, M Parrinello, ML Klein
Physical review letters 73 (23), 3133

28 1994

Molecular properties of CN⁻ ions in alkali cyanide crystals

PW Fowler, ML Klein
The Journal of chemical physics 85 (7), 3913-3916

28 1986

The crystal structure problem

KF Niebel, JA Venables, ML Klein
Rare gas solids 1, 558-589

28 1976

An atomistic model for simulations of the general anesthetic isoflurane

27 2010

J Hénin, G Brannigan, WP Dailey, R Eckenhoff, ML Klein
The Journal of Physical Chemistry B 114 (1), 604-612

Bulk and interfacial aqueous fluoride: An investigation via first principles molecular dynamics 27 2009

MH Ho, ML Klein, IFW Kuo
The Journal of Physical Chemistry A 113 (10), 2070-2074

Molecular dynamics simulations of self-assembly and nanotube formation by amphiphilic molecules in aqueous solution: a coarse-grain approach 27 2007

G Srinivas, ML Klein
Nanotechnology 18 (20), 205703

Probing the configurational space of a metalloprotein core: an ab initio molecular dynamics study of Duo Ferro 1 binuclear Zn cofactor 27 2003

GA Papoian, WF DeGrado, ML Klein
Journal of the American Chemical Society 125 (2), 560-569

Ab initio molecular dynamics study of crystal hydrates of HCl including path integral results 27 1997

T Roseninge, ME Tuckerman, ML Klein
Faraday Discussions 106, 273-289

Coupling of rotations and translations in cyanide crystals 27 1981

ML Klein, R McDonald
Chemical Physics Letters 78 (2), 383-387

Self-consistent phonon theory of rare gas solids 27 1976

NR Werthamer, ML Klein, JA Venables
Rare gas solids 1, 265-300

Analysis of the destabilization of bacterial membranes by quaternary ammonium compounds: A combined experimental and computational study 26 2020

S Alkhalifa, MC Jennings, D Granata, M Klein, WM Wuest, KPC Minbiole, ...
ChemBioChem 21 (10), 1510-1516

On the role of water density fluctuations in the inhibition of a proton channel 26 2016

E Gianti, L Delemotte, ML Klein, V Carnevale
Proceedings of the National Academy of Sciences 113 (52), E8359-E8368

Flavonoids from *Perovskia atriplicifolia* and Their in Vitro Displacement of the Respective Radioligands for Human Opioid and Cannabinoid Receptors 26 2015

A Tarawneh, F León, S Pettaway, KM Elokely, ML Klein, J Lambert, ...
Journal of natural products 78 (6), 1461-1465

Effect of the pore region of a transmembrane ion channel on the physical properties of a simple membrane 26 2004

L Saiz, S Bandyopadhyay, ML Klein
The Journal of Physical Chemistry B 108 (8), 2608-2613

- Tubular nanostructures** 26 2004
M Klein, C Lopez
US Patent App. 10/446,622
- Evolution of fragments formed at the rupture of a knotted alkane molecule** 26 1999
AM Saitta, ML Klein
Journal of the American Chemical Society 121 (50), 11827-11830
- Lattice dynamics of solid α -carbon monoxide** 26 1985
PF Fracassi, R Righini, RG Della Valle, ML Klein
Chemical physics 96 (3), 361-369
- Encapsulation of hydrophobic components in dendrimersomes and decoration of their surface with proteins and nucleic acids** 25 2019
P Torre, Q Xiao, I Buzzacchera, SE Sherman, K Rahimi, NY Kostina, ...
Proceedings of the National Academy of Sciences 116 (31), 15378-15385
- Relating Interfacial Order to Sum Frequency Generation with Ab Initio Simulations of the Aqueous $\text{Al}_2\text{O}_3(0001)$ and $(11\bar{2}0)$ Interfaces** 25 2018
M DelloStritto, SM Piontek, ML Klein, E Borguet
The Journal of Physical Chemistry C 122 (37), 21284-21294
- Self-interrupted synthesis of sterically hindered aliphatic polyamide dendrimers** 25 2017
D Jishkariani, CM MacDermaid, YN Timsina, S Grama, SS Gillani, M Divar, ...
Proceedings of the National Academy of Sciences 114 (12), E2275-E2284
- Proton transfer drives protein radical formation in *Helicobacter pylori* catalase but not in *Penicillium vitale* catalase** 25 2011
M Alfonso-Prieto, H Oberhofer, ML Klein, C Rovira, J Blumberger
Journal of the American Chemical Society 133 (12), 4285-4298
- Paramaterization of a coarse-grained model for linear alkylbenzene sulfonate surfactants and molecular dynamics studies of their self-assembly in aqueous solution** 25 2010
X He, W Shinoda, R DeVane, KL Anderson, ML Klein
Chemical Physics Letters 487 (1-3), 71-76
- The transmembrane domain of the acetylcholine receptor: insights from simulations on synthetic peptide models** 25 2005
L Saiz, ML Klein
Biophysical journal 88 (2), 959-970
- On the quantum nature of an excess proton in liquid hydrogen fluoride** 25 2004
S Raugei, ML Klein
ChemPhysChem 5 (10), 1569-1576
- Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution** 25 1998

S Bandyopadhyay, ML Klein, GJ Martyna, M Tarek
Molecular physics 95 (2), 377-384

Determination of the Pressure– Viscosity Coefficient of Decane by Molecular Simulation 25 1996

CJ Mundy, ML Klein, JI Siepmann
The Journal of Physical Chemistry 100 (42), 16779-16781

Investigation of the lattice vibrations of solid NaNO₂ by means of molecular dynamics calculations 25 1986

RM Lynden-Bell, RW Impey, ML Klein
Chemical physics 109 (1), 25-33

Interaction potentials and the properties of xenon overlayers physisorbed on the graphite basal plane 25 1984

ML Klein, S O'Shea, Y Ozaki
The Journal of Physical Chemistry 88 (7), 1420-1425

Orientational phases of a quadrupolar bilayer 25 1982

SF O'Shea, ML Klein
Physical Review B 25 (9), 5882

Molecular dynamics study of solid β -N₂ 25 1981

ML Klein, D Lévesque, JJ Weis
The Journal of Chemical Physics 74 (4), 2566-2568

Canine *CNGA3* Gene Mutations Provide Novel Insights into Human Achromatopsia-Associated Channelopathies and Treatment 24 2015

N Tanaka, EV Dutrow, K Miyadera, L Delemotte, CM MacDermaid, ...
PLoS One 10 (9), e0138943

Structural and dynamical properties of manganese catalase and the synthetic protein DF1 and their implication for reactivity from classical molecular dynamics calculations 24 2006

K Spiegel, WF De Grado, ML Klein
Proteins: Structure, Function, and Bioinformatics 65 (2), 317-330

Ab Initio Molecular Dynamics Simulation of a Water–Hydrogen Fluoride Equimolar Mixture 24 2005

C Simon, ML Klein
ChemPhysChem 6 (1), 148-153

Simulation of sodium octanoate micelles in aqueous solution 24 1991

J Shelley, K Watanabe, ML Klein
Electrochimica acta 36 (11-12), 1729-1734

A molecular dynamics study of the crystalline and liquid phases of pyridine 24 1989

Z Gamba, ML Klein
Chemical physics 130 (1-3), 15-22

- [Application of path integral simulations to the study of electron solvation in polar fluids](#) 24 1988
M Sprik, ML Klein
Computer Physics Reports 7 (3), 147-166
- [Is the ground-state structure of \(KCl\) 0.25 \(KCN\) 0.75 a noncubic orientational glass?](#) 24 1987
LJ Lewis, ML Klein
Physical review letters 59 (16), 1837
- [Molecular dynamics studies of hydrogen-bonded liquids](#) 24 1978
IR McDonald, ML Klein
Faraday Discussions of the Chemical Society 66, 48-57
- [A molecular dynamics study of the intensity and band shape of depolarized light scattered from rare-gas crystals](#) 24 1976
BJ Alder, HL Strauss, JJ Weis, JP Hansen, ML Klein
Physica B+ C 83 (3), 249-258
- [Thermodynamic Properties of Solid Argon and Krypton](#) 24 1973
ML Klein, TR Koehler, RL Gray
Physical Review B 7 (4), 1571
- [Comparison of classical Monte Carlo experiments with improved self-consistent phonon theory: Thermodynamic properties of solid Xe](#) 24 1971
ML Klein, WG Hoover
Physical Review B 4 (2), 539
- [Membrane-mimetic dendrimersomes engulf living bacteria via endocytosis](#) 23 2019
NY Kostina, K Rahimi, Q Xiao, T Haraszti, S Dedisch, JP Spatz, ...
Nano Letters 19 (8), 5732-5738
- [A hypothetical molecular mechanism for TRPV1 activation that invokes rotation of an S6 asparagine](#) 23 2018
MA Kasimova, AT Yazici, Y Yudin, D Granata, ML Klein, T Rohacs, ...
Journal of General Physiology 150 (11), 1554-1566
- [A Free-Standing Molecular Spin-Charge Converter for Ubiquitous Magnetic-Energy Harvesting and Sensing](#) 23 2017
B Xu, H Chakraborty, RC Remsing, ML Klein, S Ren
Advanced Materials 29 (8), 1605150
- [Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics](#) 23 2005
I Ivanov, ML Klein
Journal of the American Chemical Society 127 (11), 4010-4020
- [Membrane bound hydraphiles facilitate cation translocation](#) 23 2004
G Srinivas, CF Lopez, ML Klein
The Journal of Physical Chemistry B 108 (14), 4231-4235

- Ab initio molecular dynamics investigation of the formyl cation in the superacid SbF₅/HF** 23 2001
S Raugei, ML Klein
The Journal of Physical Chemistry B 105 (34), 8212-8219
- Melting transition of ethylene on graphite** 23 1992
A Cheng, ML Klein
Langmuir 8 (11), 2798-2803
- Structure of axially compressed monolayers of N₂ physisorbed on graphite** 23 1985
C Peters, ML Klein
Physical Review B 32 (9), 6077
- Effective pair potentials and the structure of ices VIII and IX** 23 1984
RW Impey, ML Klein, JS Tse
The Journal of chemical physics 81 (12), 6406-6407
- Thermodynamic properties of potassium at 160 and 308 K** 23 1975
SS Cohen, ML Klein
Physical Review B 12 (8), 2984
- Molecular motions in solid isotopic silanes** 23 1969
ML Klein, JA Morrison, RD Weir
Discussions of the Faraday Society 48, 93-101
- Magnesium-dependent RNA binding to the PA endonuclease domain of the avian influenza polymerase** 22 2014
S Xiao, ML Klein, DN LeBard, BG Levine, H Liang, CM MacDermaid, ...
The journal of physical chemistry B 118 (4), 873-889
- Facially amphiphilic polyaryl and polyaryalkynyl polymers and oligomers and uses thereof** 22 2012
WF Degrado, D Liu, GN Tew, ML Klein
US Patent 8,222,456
- Communication: Exploring the reorientation of benzene in an ionic liquid via molecular dynamics: Effect of temperature and solvent effective charge on the slow dynamics** 22 2011
Y Yasaka, ML Klein, M Nakahara, N Matubayasi
The Journal of chemical physics 134 (19), 191101
- A general purpose parallel molecular dynamics simulation program** 22 2006
KJ Oh, ML Klein
Computer physics communications 174 (7), 560-568
- Molecular dynamics simulation of a hydrated diphytanol phosphatidylcholine lipid bilayer containing an alpha-helical bundle of four transmembrane domains of the influenza A ...** 22 1999
PB Moore, DM Newns, ML Klein

Faraday Discussions 111, 200-208

- [Profile unbiased thermostat with dynamical streaming velocities](#) 22 1996
K Bagchi, S Balasubramanian, CJ Mundy, ML Klein
The Journal of chemical physics 105 (24), 11183-11189
- [Simulation of dynamical processes in molecular solids](#) 22 1990
ML Klein, LJ Lewis
Chemical Reviews 90 (3), 459-479
- [Structure of the fast-ion conducting phase of soil lithium sulphate](#) 22 1984
RW Impey, ML Klein, IR McDonald
Journal of Physics C: Solid State Physics 17 (22), 3941
- [Properties of the paraelectric-solid and molten phases of sodium nitrite](#) 22 1982
ML Klein, IR McDonald
Proceedings of the Royal Society of London. A. Mathematical and Physical ...
- [Lattice dynamics of solid ammonia](#) 22 1978
R Righini, ML Klein
The Journal of Chemical Physics 68 (12), 5553-5557
- [Lattice dynamics of hcp ortho-deuterium](#) 22 1970
ML Klein, TR Koehler
Physics Letters A 33 (4), 253-254
- [An improved self consistent phonon theory for neon](#) 22 1968
VV Goldman, GK Horton, ML Klein
Physics Letters A 28 (5), 341-342
- [New self diffusion measurements in argon gas](#) 22 1967
M De Paz, B Turi, ML Klein
Physica 36 (1), 127-135
- [Screening libraries of amphiphilic Janus dendrimers based on natural phenolic acids to discover monodisperse unilamellar dendrimersomes](#) 21 2018
I Buzzacchera, Q Xiao, H Han, K Rahimi, S Li, NY Kostina, BJ Toebes, ...
Biomacromolecules 20 (2), 712-727
- [Characterization of the honeybee AmNaV1 channel and tools to assess the toxicity of insecticides](#) 21 2015
P Gosselin-Badaroudine, A Moreau, L Delemotte, T Cens, C Collet, ...
Scientific Reports 5 (1), 1-17
- [Methods, systems, and computer program products for simulating biomembrances using coarse grain models](#) 21 2012
CF Lopez, SO Nielsen, PB Moore, ML Klein
US Patent 8,234,074

- [Hydrogen evolution from formic acid in an ionic liquid solvent: a mechanistic study by ab Initio molecular dynamics](#) 21 2011
BL Bhargava, Y Yasaka, ML Klein
The Journal of Physical Chemistry B 115 (48), 14136-14140
- [Computational study of the Zr⁴⁺ tetranuclear polymer, \[Zr₄ \(OH\)₈ \(H₂O\)₁₆\]⁸⁺](#) 21 2007
N Rao, MN Holerca, ML Klein, V Pophristic
The Journal of Physical Chemistry A 111 (45), 11395-11399
- [Ab initio molecular dynamics study of crystalline nitric acid trihydrate](#) 21 1999
DM Sullivan, K Bagchi, ME Tuckerman, ML Klein
The Journal of Physical Chemistry A 103 (43), 8678-8683
- [Nanovesicles displaying functional linear and branched oligomannose self-assembled from sequence-defined Janus glycodendrimers](#) 20 2020
Q Xiao, M Delbianco, SE Sherman, AM Reveron Perez, P Bharate, ...
Proceedings of the National Academy of Sciences 117 (22), 11931-11939
- [Toward a model for activation of Orai channel](#) 20 2019
H Dong, Y Zhang, R Song, J Xu, Y Yuan, J Liu, J Li, S Zheng, T Liu, B Lu, ...
Iscience 16, 356-367
- [Tunable two-dimensional interfacial coupling in molecular heterostructures](#) 20 2017
B Xu, H Chakraborty, VK Yadav, Z Zhang, ML Klein, S Ren
Nature communications 8 (1), 1-11
- [Morphologies of charged diblock copolymers simulated with a neutral coarse-grained model](#) 20 2011
DA Pantano, ML Klein, DE Discher, PB Moore
The Journal of Physical Chemistry B 115 (16), 4689-4695
- [Facially amphiphilic polymers and oligomers and uses thereof](#) 20 2004
WF Degrado, D Liu, GN Tew, ML Klein, J Yuan, S Choi
- [Density Functional Study of Ethylene- Norbornene Copolymerization via Metallocene and Constrained-Geometry Catalysts](#) 20 2004
EG Kim, ML Klein
Organometallics 23 (13), 3319-3326
- [First principles computational study of the active site of arginase](#) 20 2004
I Ivanov, ML Klein
Proteins: Structure, Function, and Bioinformatics 54 (1), 1-7
- [Vapor- Liquid and Vapor- Solid Phase Equilibria of Fullerenes: The Role of the Potential Shape on the Triple Point](#) 20 2003
B Chen, JI Siepmann, S Karaborni, ML Klein
The Journal of Physical Chemistry B 107 (44), 12320-12323

20 2002

- Hydrocarbon Reactivity in the Superacid SbF₅/HF: an ab Initio Molecular Dynamics Study**
S Raugei, ML Klein
The Journal of Physical Chemistry B 106 (44), 11596-11605
- Comment on" Toward a statistical thermodynamics of steady states"- Tuckerman et al. reply** 20 1998
ME Tuckerman, CJ Mundy, ML Klein
PHYSICAL REVIEW LETTERS 80 (18), 4105-4106
- High-density structures and phase transition in an ionic model of H₂O ice** 20 1989
P Demontis, ML Klein, R LeSar
Physical Review B 40 (4), 2716
- Interaction Potential of the Inert Gases** 20 1967
ML Klein, RJ Munn
The Journal of Chemical Physics 47 (3), 1035-1037
- Anharmonic contribution to the Grüneisen parameters of solid argon, krypton and xenon** 20 1967
C Feldman, JL Feldman, GK Horton, ML Klein
Proceedings of the Physical Society (1958-1967) 90 (4), 1182
- Targeting SARS-CoV-2 M3CLpro by HCV NS3/4a Inhibitors: *In Silico* Modeling and *In Vitro* Screening** 19 2021
A Manandhar, BE Blass, DJ Colussi, I Almi, M Abou-Gharbia, ML Klein, ...
Journal of chemical information and modeling 61 (2), 1020-1032
- Quantum Mechanical and Quantum Mechanical/Molecular Mechanical Studies of the Iron– Dioxygen Intermediates and Proton Transfer in Superoxide Reductase** 19 2010
PHL Sit, A Migliore, MH Ho, ML Klein
Journal of Chemical Theory and Computation 6 (9), 2896-2909
- Quadrupolar freezing in potassium bromide cyanide ((KBr) 1-x (KCN) x) mixed crystals** 19 1987
LJ Lewis, ML Klein
Journal of Physical Chemistry 91 (19), 4990-4994
- Solid and liquid carbon monoxide studied with the use of constant-pressure molecular dynamics** 19 1986
PF Fracassi, G Cardini, S O'Shea, RW Impey, ML Klein
Physical Review B 33 (5), 3441
- Phonon-orientational coupling in sodium nitrite** 19 1984
RM Lynden-Bell, ML Klein, IR McDonald
Zeitschrift für Physik B Condensed Matter 54 (4), 325-331
- Molecular dynamics calculations for solid bicyclo (2.2. 2) octane** 19 1984

E Neusy, S Nosé, ML Klein
Molecular Physics 52 (2), 269-279

[Interatomic potentials and phonon spectra of dilute rare-gas mixtures](#) 19 1974
SS Cohen, ML Klein
The Journal of Chemical Physics 61 (8), 3210-3216

[Perturbation theory of anharmonic crystals](#) 19 1974
THK Barron, ML Klein
NATIONAL RESEARCH COUNCIL OF CANADA OTTAWA (ONTARIO)

[Comments on the interatomic potential of Ne₂](#) 19 1973
ML Klein
Chemical Physics Letters 18 (2), 203-204

[A coarse-grain model for entangled polyethylene melts and polyethylene crystallization](#) 18 2019
KW Hall, TW Sirk, ML Klein, W Shinoda
The Journal of Chemical Physics 150 (24), 244901

[Unknotting of a polymer strand in a melt](#) 18 2004
EG Kim, ML Klein
Macromolecules 37 (5), 1674-1677

[Molecular dynamics studies of titanylphthalocyanine crystals](#) 18 1996
O Okada, ML Klein
Journal of the Chemical Society, Faraday Transactions 92 (13), 2463-2467

[A molecular dynamics study of n-hexadecane droplets on a hydrophobic surface](#) 18 1994
W Mar, ML Klein
Journal of Physics: Condensed Matter 6 (23A), A381

[Gas-surface potentials and the dynamics of overlayers](#) 18 1985
G Cardini, SF O'Shea, ML Klein
Faraday discussions of the Chemical Society 80, 227-238

[The elastic constants of solid Ar](#) 18 1973
TG Gibbons, ML Klein, RD Murphy
Chemical Physics Letters 18 (3), 325-328

[Scattering measurements, second virial coefficients, and the interatomic potential for argon](#) 18 1971
JA Barker, ML Klein
Chemical Physics Letters 11 (4), 501-503

[Modeling liquid water by climbing up Jacob's ladder in density functional theory facilitated by using deep neural network potentials](#) 17 2021
C Zhang, F Tang, M Chen, J Xu, L Zhang, DY Qiu, JP Perdew, ML Klein, ...
The Journal of Physical Chemistry B 125 (41), 11444-11456

- TRPA1 modulation by piperidine carboxamides suggests an evolutionarily conserved binding site and gating mechanism** 17 2019
T Chernov-Rogan, E Gianti, C Liu, E Villemure, AP Cridland, X Hu, ...
Proceedings of the National Academy of Sciences 116 (51), 26008-26019
- Characterization of Membrane-Protein Interactions for the Leucine Transporter from *Aquifex aeolicus* by Molecular Dynamics Calculations** 17 2009
DA Pantano, ML Klein
The Journal of Physical Chemistry B 113 (42), 13715-13722
- Ab initio calculations of intramolecular parameters for a class of arylamide polymers** 17 2006
S Vemparala, I Ivanov, V Pophristic, K Spiegel, ML Klein
Journal of computational chemistry 27 (6), 693-700
- Molecular dynamics simulation of four- α -helix bundles that bind the anesthetic halothane** 17 2000
LA Davies, Q Zhong, ML Klein, D Scharf
Febs Letters 478 (1-2), 61-66
- Molecular dynamics simulation of a synthetic four- α -helix bundle that binds the anesthetic halothane** 17 1999
LA Davies, ML Klein, D Scharf
FEBS letters 455 (3), 332-338
- Trimethylaluminum: a computer study of the condensed phases and the gas dimer** 17 1998
S Balasubramanian, CJ Mundy, ML Klein
The Journal of Physical Chemistry B 102 (50), 10136-10141
- Response to "Comment on 'Modified nonequilibrium molecular dynamics for fluid flows with energy conservation'" [J. Chem. Phys. **108**, 4351 (1998)]** 17 1998
ME Tuckerman, CJ Mundy, S Balasubramanian, ML Klein
The Journal of chemical physics 108 (10), 4353-4354
- Molecular dynamics studies of microscopic wetting phenomena on self-assembled monolayers** 17 1995
W Mar, J Hautman, ML Klein
Computational materials science 3 (4), 481-497
- C 60 O: a molecular dynamics study of rotation in the solid phase solid phase** 17 1992
A Cheng, ML Klein
Journal of the Chemical Society, Faraday Transactions 88 (14), 1949-1951
- Molecular dynamics investigation of alkali-metal-doped fullerites** 17 1991
A Cheng, ML Klein
The Journal of Physical Chemistry 95 (24), 9622-9625

- The continuous melting transition of ethylene on graphite: a molecular dynamics study** 17 1989
MA Moller, ML Klein
Chemical physics 129 (2), 235-239
- Dispersion of surface phonons in a xenon monolayer physisorbed on the graphite basal plane** 17 1984
M Marchese, G Jacucci, ML Klein
Surface science 145 (2-3), 364-370
- Mol. Phys.** 17 1984
S Nose, ML Klein
- Relationship between Adiabatic Elastic Constants and the Slopes of Phonon Dispersion Curves for Rare-Gas Solids** 17 1971
VV Goldman, GK Horton, ML Klein
Physical Review B 4 (2), 567
- Direct visualization of vesicle disassembly and reassembly using photocleavable dendrimers elucidates cargo release mechanisms** 16 2020
S Li, B Xia, B Javed, WD Hasley, A Melendez-Davila, M Liu, M Kerzner, ...
Acs Nano 14 (6), 7398-7411
- Sodium halide adsorption and water structure at the α -alumina (0001)/water interface** 16 2019
R Wang, M DelloStritto, RC Remsing, V Carnevale, ML Klein, E Borguet
The Journal of Physical Chemistry C 123 (25), 15618-15628
- Effect of Functional and Electron Correlation on the Structure and Spectroscopy of the $\text{Al}_2\text{O}_3(001)\text{-H}_2\text{O}$ Interface** 16 2019
MJ DelloStritto, SM Piontek, ML Klein, E Borguet
The Journal of Physical Chemistry Letters 10 (9), 2031-2036
- Rotational dynamics of benzene and water in an ionic liquid explored via molecular dynamics simulations and NMR T_1 measurements** 16 2012
Y Yasaka, ML Klein, M Nakahara, N Matubayasi
The Journal of Chemical Physics 136 (7), 074508
- Incorporating a hydrophobic solid into a coarse grain liquid framework: Graphite in an aqueous amphiphilic environment** 16 2005
SO Nielsen, G Srinivas, ML Klein
The Journal of chemical physics 123 (12), 124907
- Static disorder in the mixed crystals (KCN) x (KBr) $1-x$ and its relation to dynamical properties** 16 1982
DG Bounds, ML Klein, IR McDonald, Y Ozaki
Molecular Physics 47 (3), 629-636

- Molecular dynamics calculations for solid and liquid acetylene** 16 1981
ML Klein, IR McDonald
Chemical Physics Letters 80 (1), 76-82
- Molecular dynamics study of solid nitrogen at high pressure** 16 1981
ML Klein, D Levesque, JJ Weis
Canadian Journal of Physics 59 (4), 530-534
- Comparison of Classical Monte Carlo Experiments with Self-Consistent Phonon Theory: Elastic Constants for Solid Xenon** 16 1971
ML Klein, WG Hoover
Physical Review B 4 (2), 537
- Phonon energies and lifetimes in solid argon near 0 degrees K** 16 1970
VV Goldman, GK Horton, TH Keil, ML Klein
Journal of Physics C: Solid State Physics 3 (1), L33
- Anharmonic Forces and the Vapor-Pressure Ratio of Monatomic Isotopic Solids** 16 1964
ML Klein
The Journal of Chemical Physics 41 (3), 749-755
- Science 1997, 275, 817- 820** 16
ME Tuckerman, D Marx, ML Klein, M Parrinello
Google Scholar There is no corresponding record for this reference
- Aqueous solvation of the chloride ion revisited with density functional theory: impact of correlation and exchange approximations** 15 2020
M DelloStritto, J Xu, X Wu, ML Klein
Physical Chemistry Chemical Physics 22 (19), 10666-10675
- X-ray absorption of liquid water by advanced *ab initio* methods** 15 2017
Z Sun, M Chen, L Zheng, J Wang, B Santra, H Shen, L Xu, W Kang, ...
Physical Review B 96 (10), 104202
- Proton release from the histidine-tetrad in the M2 channel of the influenza A virus** 15 2014
H Dong, G Fiorin, WF DeGrado, ML Klein
The Journal of Physical Chemistry B 118 (44), 12644-12651
- Exploring histidine conformations in the M2 channel lumen of the influenza A virus at neutral pH via molecular simulations** 15 2013
H Dong, G Fiorin, WF DeGrado, ML Klein
The journal of physical chemistry letters 4 (18), 3067-3071
- Proton affinity of the histidine-tryptophan cluster motif from the influenza A virus from *ab initio* molecular dynamics** 15 2013
A Bankura, ML Klein, V Carnevale
Chemical physics 422, 156-164

- Hydrodynamic boundary conditions for confined fluids via a nonequilibrium molecular dynamics simulation** 15 1996
CJ Mundy, S Balasubramanian, ML Klein
The Journal of chemical physics 105 (8), 3211-3214
- Molecular dynamics study of solid argon with N₂, O₂, and CO impurities** 15 1982
S Nosé, ML Klein
Canadian Journal of Physics 60 (9), 1365-1370
- Phonon spectra of methane physisorbed on graphite** 15 1981
K Maki, ML Klein
The Journal of Chemical Physics 74 (2), 1488-1494
- A molecular dynamics study of the lattice vibrations of sodium chloride** 15 1975
G Jacucci, ML Klein, IR McDonald
Journal de Physique Lettres 36 (4), 97-100
- Enhanced concanavalin A binding to preorganized mannose nanoarrays in glycodendrimersomes revealed multivalent interactions** 14 2021
N Yu. Kostina, D Söder, T Haraszti, Q Xiao, K Rahimi, BE Partridge, ...
Angewandte Chemie 133 (15), 8433-8441
- First-Principles Calculation of Water pK_a Using the Newly Developed SCAN Functional** 14 2019
R Wang, V Carnevale, ML Klein, E Borguet
The Journal of Physical Chemistry Letters 11 (1), 54-59
- Suppression of zika virus infection in the brain by the antiretroviral drug rilpivirine** 14 2019
IK Sariyer, J Gordon, TH Burdo, HS Wollebo, E Gianti, M Donadoni, ...
Molecular Therapy 27 (12), 2067-2079
- Light-induced dilation in nanosheets of charge-transfer complexes** 14 2018
Z Zhang, RC Remsing, H Chakraborty, W Gao, G Yuan, ML Klein, S Ren
Proceedings of the National Academy of Sciences 115 (15), 3776-3781
- Counterion-assisted cation transport in a biological calcium channel** 14 2014
H Dong, ML Klein, G Fiorin
The Journal of Physical Chemistry B 118 (32), 9668-9676
- Modeling lipid membranes** 14 2005
C Chipot, ML Klein, M Tarek
Handbook of materials modeling, 929-958
- Intramolecular hydrogen bonds: ab initio Car-Parrinello simulations of arylamide torsions** 14 2003
RJ Doerksen, B Chen, ML Klein
Chemical physics letters 380 (1-2), 150-157

- Structure and electrostatics of the surfactant-water interface** 14 1997
JC Shelley, M Sprik, ML Klein
Amphiphiles at Interfaces, 146-154
- Orientational ordering in mixed cyanide crystals:(NaCN) 1– x (KCN) x** 14 1991
A Cheng, ML Klein, LJ Lewis
Physical Review B 44 (1), 13
- Molecular-dynamics studies of the mixed cyanides. II. Orientational freezing** 14 1989
LJ Lewis, ML Klein
Physical Review B 40 (10), 7080
- Orientational ordering in solid parahydrogen and orthodeuterium** 14 1984
M Sprik, ML Klein
The Journal of chemical physics 81 (12), 6207-6213
- Y. Ozaki and IR McDonald** 14 1982
ML Klein
J. Phys. C 15, 4993
- Solvation dynamics in water confined within layered manganese dioxide** 13 2017
RC Remsing, ML Klein
Chemical Physics Letters 683, 478-482
- SCAN: An efficient density functional yielding accurate structures and energies of diversely-bonded materials** 13 2015
J Sun, RC Remsing, Y Zhang, Z Sun, A Ruzsinszky, H Peng, Z Yang, ...
arXiv preprint arXiv:1511.01089
- Computer simulations of voltage-gated cation channels** 13 2012
W Treptow, ML Klein
The journal of physical chemistry letters 3 (8), 1017-1023
- Effects of halothane on Dimyristoylphosphatidylcholine lipid bilayer structure: a molecular dynamics simulation study** 13 2009
KJ Oh, ML Klein
Bulletin of the Korean Chemical Society 30 (9), 2087-2092
- A simple protocol for identification of helical and mobile residues in membrane proteins** 13 1995
DJ Tobias, J Gesell, ML Klein, SJ Opella
Journal of molecular biology 253 (3), 391-395
- Electronic states and the metal–insulator transition in caesium–ammonia solutions** 13 1994
Z Deng, ML Klein, GJ Martyna
Journal of the Chemical Society, Faraday Transactions 90 (14), 2009-2013
- Molecular dynamics simulation of Pf1 coat protein** 13 1993
DJ Tobias, ML Klein, SJ Opella

Biophysical journal 64 (3), 670-675

Molecular dynamics study of a model Langmuir-Blodgett film 13 1988
 JP Bareman, G Cardini, ML Klein
 MRS Online Proceedings Library (OPL) 141

Structure of the nitrite ion 13 1983
 JD Goddard, ML Klein
 Physical Review A 28 (2), 1141

Lattice vibrations of solid α -F2 13 1980
 K Kobashi, ML Klein
 Molecular Physics 41 (3), 679-688

Anharmonic Forces and the Vapor-Pressure Ratio of Monatomic Isotopic Solids. II 13 1964
 ML Klein, JA Reissland
 The Journal of Chemical Physics 41 (9), 2773-2776

Polymer nucleation under high-driving force, long-chain conditions: Heat release and the separation of time scales 12 2019
 KW Hall, S Percec, ML Klein
 The Journal of Chemical Physics 150 (11), 114901

Defect-enriched tunability of electronic and charge-carrier transport characteristics of 2D borocarbonitride (BCN) monolayers from ab initio calculations 12 2019
 VK Yadav, H Chakraborty, ML Klein, UV Waghmare, CNR Rao
 Nanoscale 11 (41), 19398-19407

Propofol inhibits the voltage-gated sodium channel NaChBac at multiple sites 12 2018
 Y Wang, E Yang, MM Wells, V Bondarenko, K Woll, V Carnevale, ...
 Journal of General Physiology 150 (9), 1317-1331

Bioactivity-Guided Isolation of Potential Antidiabetic and Antihyperlipidemic Compounds from *Trigonella stellata* 12 2018
 SM Shams Eldin, MM Radwan, AS Wanas, AAM Habib, FF Kassem, ...
 Journal of natural products 81 (5), 1154-1161

Phonons and thermal conducting properties of borocarbonitride (BCN) nanosheets 12 2018
 H Chakraborty, S Mogurampelly, VK Yadav, UV Waghmare, ML Klein
 Nanoscale 10 (47), 22148-22154

Understanding the self-assembly of amino ester-based benzene-1, 3, 5-tricarboxamides using molecular dynamics simulations 12 2017
 KK Bejagam, RC Remsing, ML Klein, S Balasubramanian
 Physical Chemistry Chemical Physics 19 (1), 258-266

- Combined computational and experimental analysis of a complex of ribonuclease III and the regulatory macrodomain protein, YmdB** 12 2015
S Paudyal, M Alfonso-Prieto, V Carnevale, SK Redhu, ML Klein, ...
Proteins: Structure, Function, and Bioinformatics 83 (3), 459-472
- Effective interaction between small unilamellar vesicles as probed by coarse-grained molecular dynamics simulations** 12 2014
W Shinoda, ML Klein
Pure and Applied Chemistry 86 (2), 215-222
- Computing the acidity of liquids via Ab initio molecular dynamics** 12 2007
C Simon, G Ciccotti, ML Klein
ChemPhysChem 8 (14), 2072-2076
- Phase transition and water molecules in titanylphthalocyanine phase Y crystal** 12 2001
O Okada, ML Klein
Physical Chemistry Chemical Physics 3 (8), 1530-1534
- Translation-rotation coupling and the lattice dynamics of solid carbon monoxide** 12 1984
PF Fracassi, ML Klein
Chemical physics letters 108 (4), 359-362
- Effect of changes in pair potential on the dynamical structure factor of molecular crystals** 12 1980
CS Murthy, K Singer, ML Klein, IR McDonald
Molecular Physics 40 (6), 1517-1521
- Models for strongly polar liquids** 12 1980
GN Patey, ML Klein, IR McDonald
Chemical Physics Letters 73 (2), 375-377
- Anharmonic phonon response in aluminum: A neutron-scattering test of computer-simulation calculations** 12 1979
WJL Buyers, G Dolling, G Jacucci, ML Klein, HR Glyde
Physical Review B 20 (12), 4859
- Probing Heterogeneous Charge Distributions at the α -Al₂O₃(0001)/H₂O Interface** 11 2020
SM Piontek, M DelloStritto, B Mandal, T Marshall, ML Klein, E Borguet
Journal of the American Chemical Society 142 (28), 12096-12105
- Chemical physics of water** 11 2017
PG Debenedetti, ML Klein
Proceedings of the National Academy of Sciences 114 (51), 13325-13326
- Exploring the complex dynamics of an ion channel voltage sensor domain** 11 2017

via computation

L Delemotte, MA Kasimova, D Sigg, ML Klein, V Carnevale, M Tarek
 BioRxiv, 108217

Dehydration of multilamellar fatty acid membranes: Towards a computational model of the stratum corneum 11 2014

CM MacDermaid, RH DeVane, ML Klein, G Fiorin
 The Journal of Chemical Physics 141 (22), 12B628_1

A cyclic nucleotide-gated channel mutation associated with canine daylight blindness provides insight into a role for the S2 segment tri-Asp motif in channel biogenesis 11 2014

N Tanaka, L Delemotte, ML Klein, AM Komáromy, JC Tanaka
 PLoS One 9 (2), e88768

Facially amphiphilic polymers and oligomers and uses thereof 11 2013

WF DeGrado, GN Tew, ML Klein, D Liu, J Yuan, S Choi
 US Patent 8,455,490

Novel conformationally-constrained β -peptides characterized by 1H NMR chemical shifts 11 2003

RJ Doerksen, B Chen, J Yuan, JD Winkler, ML Klein
 Chemical communications, 2534-2535

Ab initio study of BF_3^+ (HF) 1–7 clusters 11 1999

D Kim, ML Klein
 Chemical physics letters 308 (3-4), 235-241

Computation of the hydrodynamic boundary parameters of a confined fluid via non-equilibrium molecular dynamics 11 1997

CJ Mundy, S Balasubramanian, ML Klein
 Physica A: Statistical Mechanics and its Applications 240 (1-2), 305-314

Molecular-dynamics studies of the mixed cyanides: I. Structural transformations 11 1989

LJ Lewis, ML Klein
 Physical Review B 40 (7), 4877

Structure of solid *t*-butyl cyanide: A study by means of constant-temperature, constant-pressure, molecular-dynamics simulations 11 * 1987

M Ferrario, ML Klein, IR McDonald
 The Journal of chemical physics 87 (8), 4823-4828

Intermolecular force models and the crystal structure of carbon disulphide 11 1983

RW Impey, ML Klein
 Chemical physics letters 103 (2), 143-146

Molecular dynamics calculations for HCl in a matrix of solid Ar 11 1982

S Nosé, ML Klein
 Molecular Physics 46 (5), 1063-1071

- Localized modes in Rb-K alloys** 11 1977
G Jacucci, ML Klein, R Taylor
Solid State Communications 24 (9), 685-686
- Three-body interactions and lattice sums in crystals** 11 1971
JA Barker, ML Klein, MV Bobetic, IJ Zucker, MB Doran, GG Chell
Journal of Physics C: Solid State Physics 4 (17), L355
- Probing sulfatide-tissue lectin recognition with functionalized glycodendrimersomes** 10 2021
PV Murphy, A Romero, Q Xiao, AK Ludwig, S Jogula, NV Shilova, T Singh, ...
Iscience 24 (1), 101919
- Lone pair rotational dynamics in solids** 10 2020
RC Remsing, ML Klein
Physical review letters 124 (6), 066001
- Losing supramolecular orientational memory via self-organization of a misfolded secondary structure** 10 2018
D Sahoo, M Peterca, E Aqad, BE Partridge, ML Klein, V Percec
Polymer Chemistry 9 (18), 2370-2381
- Small molecule modulation of voltage gated sodium channels** 10 2017
V Carnevale, ML Klein
Current opinion in structural biology 43, 156-162
- Probing the dynamics of N-methylacetamide in methanol via ab initio molecular dynamics** 10 2017
VK Yadav, ML Klein
Physical Chemistry Chemical Physics 19 (20), 12868-12875
- A study of longitudinal tumor motion in helical tomotherapy using a cylindrical phantom** 10 2013
M Klein, S Gaede, S Yartsev
Journal of Applied Clinical Medical Physics 14 (2), 52-61
- A parallel molecular dynamics simulation scheme for a molecular system with bond constraints in NPT ensemble** 10 2006
KJ Oh, ML Klein
Computer physics communications 174 (4), 263-269
- Structure of the strongly associated liquid antimony pentafluoride: An *ab initio* molecular dynamics study** 10 2002
S Raugei, ML Klein
The Journal of chemical physics 116 (16), 7087-7093
- Influence of a knot on the stretching-induced crystallization of a polymer** 10 2002
AM Saitta, ML Klein
The Journal of chemical physics 116 (13), 5333-5336

- [Short-range structure of liquid pyrrole](#) 10 1990
Z Gamba, ML Klein
The Journal of chemical physics 92 (11), 6973-6974
- [Calculation of the molar volume of electron solvation in liquid ammonia](#) 10 1990
M Marchi, M Sprik, ML Klein
Journal of Physical Chemistry 94 (1), 431-434
- [Erratum: Optimization of a distributed Gaussian basis set using simulated annealing: Application to the adiabatic dynamics of the solvated electron \[J. Chem. Phys. 89, 1592 ...\]](#) 10 1989
M Sprik, ML Klein
The Journal of Chemical Physics 90 (12), 7614-7614
- [A computer simulation study of supercooled liquid and amorphous-solid methanol](#) 10 1989
M Marchi, ML Klein
Zeitschrift für Naturforschung A 44 (6), 585-590
- [Structure and dynamics of the fluorperovskite, RbCaF₃](#) 10 1989
S Nosé, ML Klein
The Journal of chemical physics 90 (9), 5005-5010
- [Calculation of the free energy of electron solvation in liquid ammonia using a path integral quantum Monte Carlo simulation](#) 10 1988
M Marchi, M Sprik, ML Klein
The Journal of Physical Chemistry 92 (12), 3625-3629
- [A molecular dynamics study of the rotator phase of t-butyl bromide](#) 10 1987
M Ferrario, ML Klein, RM Lynden-Bell, IR McDonald
Journal of the Chemical Society, Faraday Transactions 2: Molecular and ...
- [Dynamical structure factor \$S\(Q, \omega\)\$ of solid potassium](#) 10 1976
JP Hansen, ML Klein
Solid State Communications 20 (8), 771-773
- [Self-consistent phonon calculation of the elastic constants of the \$\beta\$ phase of solid N₂](#) 10 1976
VV Goldman, ML Klein
The Journal of Chemical Physics 64 (12), 5121-5125
- [Importance of nuclear quantum effects on the hydration of chloride ion](#) 9 2021
J Xu, Z Sun, C Zhang, M DelloStritto, D Lu, ML Klein, X Wu
Physical Review Materials 5 (1), L012801
- [Unraveling topology-induced shape transformations in dendrimersomes](#) 9 2021
NY Kostina, AM Wagner, T Haraszti, K Rahimi, Q Xiao, ML Klein, V Percec, ...
Soft Matter 17 (2), 254-267

- Property decoupling across the embryonic nucleus–melt interface during polymer crystal nucleation** 9 2020
KW Hall, S Percec, W Shinoda, ML Klein
The Journal of Physical Chemistry B 124 (23), 4793-4804
- A new perspective on lone pair dynamics in halide perovskites** 9 2020
RC Remsing, ML Klein
APL Materials 8 (5), 050902
- Divining the shape of nascent polymer crystal nuclei** 9 2019
KW Hall, TW Sirk, S Percec, ML Klein, W Shinoda
The Journal of Chemical Physics 151 (14), 144901
- Bioactive products from singlet oxygen photooxygenation of cannabinoids** 9 2018
AG Osman, KM Elokely, VK Yadav, P Carvalho, M Radwan, D Slade, ...
European Journal of Medicinal Chemistry 143, 983-996
- ertes, S.** 9 2015
S Zhang, RO Moussodia, C Murzeau, HJ Sun, ML Klein
Andr' e, R. Roy, HJ Gabius and V. Percec, Angew. Chem 127, 4108
- Intermolecular Motion in Solid C70: A Molecular Dynamics Simulation Study** 9 1994
M Sprik, ML Klein
The Journal of Physical Chemistry 98 (37), 9297-9300
- Orientational ordering in the solid fullerene oxide: C60O** 9 1994
A Cheng, ML Klein
Journal of the Chemical Society, Faraday Transactions 90 (2), 253-261
- Competing interactions in self-assembled monolayers containing peptide groups: Molecular dynamics studies of long-chain perfluoro mercaptans on Au (111)** 9 1994
U Röthlisberger, ML Klein, M Sprik
Journal of Materials Chemistry 4 (6), 793-803
- Infrared and Raman spectra of hexagonal ice in the lattice-mode region** 9 1987
M Marchi, ST John, ML Klein
Journal of the Chemical Society, Faraday Transactions 2: Molecular and ...
- Gas-surface potentials and the interpretation of experiments on the ethylene/graphite system using molecular dynamics calculations** 9 1987
ML Klein, JA Morrison
Carbon 25 (1), 23-30
- Lattice dynamics of ionic molecular crystals in the rigid ion approximation, phases II and III of sodium superoxide** 9 1984
PF Fracassi, ML Klein, RG Della Valle
Canadian journal of physics 62 (1), 54-64

- Molecular-dynamics study of phase I of RbCN** 9 1981
DG Bounds, ML Klein, IR McDonald
Physical Review B 24 (6), 3568
- Structure and dynamics of associated molecular systems. IV. The orientationally disordered phase I of solid DCI** 9 1980
IR McDonald, DG Bounds, ML Klein
The Journal of Chemical Physics 73 (1), 532-537
- A Monte Carlo computer simulation of the thermodynamic properties of solid N₂** 9 1974
TG Gibbons, ML Klein
Chemical Physics Letters 29 (3), 463-465
- Monte Carlo Study of the Elastic Constants of Compressed Ar** 9 1972
ML Klein
Physical Review B 6 (10), 4082
- Volume dependence of self consistent phonon energies** 9 1970
ML Klein, GG Chell, VV Goldman, GK Horton
Journal of Physics C: Solid State Physics 3 (4), 806
- Calculation of the Vapor-Pressure Ratio of the Isotopes of Solid Ne and Ar** 9 1970
ML Klein, W Blizard, VV Goldman
The Journal of Chemical Physics 52 (4), 1633-1635
- Investigations of water/oxide interfaces by molecular dynamics simulations** 8 2021
R Wang, ML Klein, V Carnevale, E Borguet
Wiley Interdisciplinary Reviews: Computational Molecular Science 11 (6), e1537
- Effect of water frustration on water oxidation catalysis in the nanoconfined interlayers of layered manganese oxides birnessite and busserite** 8 2021
RK Bhullar, MJ Zdilla, ML Klein, RC Remsing
Journal of Materials Chemistry A 9 (11), 6924-6932
- Monodisperse polymer melts crystallize via structurally polydisperse nanoscale clusters: insights from polyethylene** 8 2020
KW Hall, TW Sirk, S Percec, ML Klein, W Shinoda
Polymers 12 (2), 447
- Tunable catalytic activity of cobalt-intercalated layered MnO₂ for water oxidation through confinement and local ordering** 8 2019
J Ning, JW Furness, Y Zhang, AC Thenuwara, RC Remsing, ML Klein, ...
Journal of Catalysis 374, 143-149
- Refined description of liquid and supercooled silicon from *ab initio* simulations** 8 2018
RC Remsing, ML Klein, J Sun
Physical Review B 97 (14), 140103

- Intramolecular hydrogen bonding appetency for conformational penchants in oxalohydrazide fluoro derivatives: NMR, MD, QTAIM, and NCI studies** 8 2018
A Lakshmipriya, M Chaudhary, S Mogurampelly, ML Klein, ...
The Journal of Physical Chemistry A 122 (10), 2703-2713
- Understanding the Boron–Nitrogen Interaction and Its Possible Implications in Drug Design** 8 2015
H Dong, W Li, J Sun, S Li, ML Klein
The Journal of Physical Chemistry B 119 (45), 14393-14401
- New Glycosides and Trypanocidal Metabolites from *Vangueria edulis*** 8 2015
SMM Mohamed, KM Elokely, EY Bachkeet, SAL Bayoumi, V Carnevale, ...
Natural product communications 10 (11), 1934578X1501001121
- Competing interactions and orientational ordering in (NaCN) 1– x (KCN) x quadrupolar glasses** 8 1991
A Cheng, ML Klein, LJ Lewis
Physical review letters 66 (5), 624
- Dispersion of surface phonons in xenon overlayers physisorbed on the Ag (111) surface** 8 1985
GG Cardini, SF O'Shea, M Marchese, ML Klein
Physical Review B 32 (6), 4261
- Lattice dynamics of the high-pressure monoclinic phase of solid carbon tetrachloride** 8 1982
R Righini, ML Klein
Chemical Physics Letters 87 (6), 604-606
- Comment on the structure of liquid ammonia** 8 1981
ML Klein, IR McDonald
The Journal of Chemical Physics 74 (7), 4214-4215
- Lattice dynamics of solid Ne** 8 1976
VV Goldman, ML Klein
Journal of Low Temperature Physics 22 (5), 501-506
- Neutron and Brillouin Scattering in Quantum Crystals** 8 1970
GK Horton, VV Goldman, ML Klein
Journal of Applied Physics 41 (13), 5138-5140
- EQUATION OF STATE OF SOLID AR KR XE** 8 1968
ML Klein, GK Horton, JL Feldman
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 13 (4), 689-&
- Interactions between physically adsorbed molecules** 8 1967
JD Johnson, ML Klein
Transactions of the Faraday Society 63, 1269-1273
- Coexistence of lipid phases stabilizes interstitial water in the outer layer of** 7 2020

mammalian skin

CM MacDermid, KW Hall, RH DeVane, ML Klein, G Fiorin
Biophysical journal 118 (7), 1588-1601

Halogen bond structure and dynamics from molecular simulations

RC Remsing, ML Klein
The Journal of Physical Chemistry B 123 (29), 6266-6273

Effect of Interlayer Co^{2+} on Structure and Charge Transfer in NiFe Layered Double Hydroxides

MJ DelloStritto, AC Thenuwara, ML Klein, DR Strongin
The Journal of Physical Chemistry C 123 (22), 13593-13599

Bonding in the metallic molecular solid α -Gallium

RC Remsing, J Sun, UV Waghmare, ML Klein
Molecular Physics 116 (21-22), 3372-3379

Simple facially amphiphilic polymers as peptide mimics.

GN Tew, WF DeGrado, ML Klein, DH Lui
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 224, U52-U52

Effects of particle size fluctuations in a breathing Lennard-Jones liquid

J Hautman, ML Klein
Molecular Physics 80 (3), 647-654

Lattice dynamics of KCN and NaCN in the antiferroelectric phase III

PF Fracassi, ML Klein
Canadian journal of physics 62 (8), 725-729

A correlated variational wave function for the orientational ground state of solid methane

M Sprik, ML Klein
The Journal of chemical physics 80 (5), 1988-1999

Infrared absorption in doped rare gas crystals

J Vermesse, D Levesque, JJ Weis, ML Klein
Canadian journal of physics 61 (11), 1545-1548

Radial correlations in associated liquids

ML Klein, IR McDonald, BJ Berne, M Rao, DL Beveridge, PK Mehrotra
The Journal of Chemical Physics 71 (9), 3889-3891

Anharmonic lattice dynamics of solid Al

G Jacucci, ML Klein
Physical Review B 16 (4), 1322

Rare gas solids. 2 (1977)

ML Klein
Academic Press

7 2019

7 2019

7 2018

7 2002

7 1993

7 1984

7 1984

7 1983

7 1979

7 1977

7 1977

- Computer «experiments» on solid rare gases: the dynamical structure factor $S(Q, \omega)$** 7 1974
JP Hansen, ML Klein
Journal de Physique Lettres 35 (3), 29-31
- Computer simulation of self-assembling macromolecules** 6 2013
G Fiorin, ML Klein, R DeVane, W Shinoda
Hierarchical Macromolecular Structures: 60 Years after the Staudinger Nobel ...
- THE ROYAL SOCIETY OF CHEMISTRY** 6 2005
PJ Sarre, IWM Smith, MNR Ashfold, DC Clary, LR Fisher, HM Frey, ...
- Proton tunneling in fatty acid/soap crystals?** 6 2003
AM Saitta, ML Klein
The Journal of chemical physics 118 (1), 1-3
- A coarse grain model for lipid monolayer and bilayer studies** 6 2002
SO Nielsen, ML Klein
Bridging Time Scales: Molecular Simulations for the Next Decade, 27-63
- Dynamical Properties of Solids** 6 1990
LJ Lewis, ML Klein, GK Horton, AA Maradudin
Elsevier, Amsterdam
- The low temperature structure of ethylene monolayers physisorbed on the graphite basal plane** 6 1988
MA Moller, ML Klein
Canadian journal of chemistry 66 (4), 774-778
- Structure and dynamics of molecular crystals** 6 1985
ML Klein
Proc. Int. School of Phys., 424-476
- Calculation of phonons in the pyrite phases of sodium superoxide** 6 1983
PF Fracassi, ML Klein
Physical Review B 28 (2), 997
- 'Lattice Dynamics of Rare Gas Solids** 6 1976
ML Klein, TR Koehler
Rare Gas Solids I, 301-381
- On the velocity of sound in solid argon** 6 1967
C Feldman, ML Klein
Physics Letters A 25 (3), 190-191
- Proc. Phys. Soc.** 6 1965
THK Barron, ML Klein
- Different bonding type along each crystallographic axis: Computational** 5 2020

[study of poly\(*p*-phenylene terephthalamide\)](#)

J Yu, G Fiorin, H Peng, ML Klein, JP Perdew
Physical Review Materials 4 (5), 055601

[Molecular simulation of covalent bond dynamics in liquid silicon](#)

RC Remsing, ML Klein
The Journal of Physical Chemistry B 124 (15), 3180-3185

[Mechanically strong polymer sheets from aligned ultrahigh-molecular-weight polyethylene nanocomposites](#)

Z Zhang, S Mogurampelly, S Percec, Y Hu, G Fiorin, ML Klein, S Ren
The Journal of Physical Chemistry Letters 9 (10), 2652-2658

[A consistent picture of TRPV1 activation emerges from molecular simulations and experiments](#)

MA Kasimova, AT Yazici, Y Yudin, D Granata, ML Klein, T Rohacs, ...
Biorxiv, 310151

[TRPV1 activation relies on hydration/dehydration of nonpolar cavities](#)

MA Kasimova, A Yazici, Y Yudin, D Granata, ML Klein, T Rohacs, ...
bioRxiv, 114546

[Coarse grained to atomistic mapping algorithm: a tool for multiscale simulations](#)

SO Nielsen, B Ensing, PB Moore, ML Klein
Multiscale simulation methods for nanomaterials, 73-88

[Application of Density Functional Theory Based Car-Parrinello Simulations to the Study of Catalytic Processes](#)

S Raugei, D Kim, ML Klein
Quantitative Structure-Activity Relationships 21 (2), 149-165

[Molecular dynamics study of structure and gating of low molecular weight ion channels](#)

DM News, Q Zhong, PB Moore, T Husslein, P Pattnaik, ML Klein
Parallel Computing 26 (7-8), 965-976

[Tuckerman *et al.* Reply:](#)

ME Tuckerman, CJ Mundy, ML Klein
Physical Review Letters 80 (18), 4105

[Erratum: Decane under shear: A molecular dynamics study using reversible NVT-SLLOD and NPT-SLLOD algorithms \[J. Chem. Phys. **103**, 10192 \(1995\)\]](#)

CJ Mundy, JI Siepmann, ML Klein
The Journal of Chemical Physics 104 (19), 7797-7797

[Ab initio simulation of the structure and dynamics of white phosphorus \(P₄\) at low temperatures](#)

PJ Ungar, K Laasonen, ML Klein

Canadian journal of physics 73 (11-12), 710-717

Molecular dynamics simulation of a langmuir monolayer 5 1991
JP Bareman, ML Klein
MRS Online Proceedings Library (OPL) 237

Ab initio interatomic potential curves for NaNO₂ and the simulation of the molten salt 5 1983
J D. Goddard, M L. Klein, Y Ozaki
Journal of the Physical Society of Japan 52 (4), 1168-1172

Hydrogen atoms in solid Ar 5 1977
SS Cohen, ML Klein
The Journal of Chemical Physics 67 (5), 2396-2397

Comments on the claimed difference between the thermal and elastic Debye temperatures of copper near 0° K 5 1972
ML Klein, DL Martin
Physics Letters A 38 (6), 430

Co-assembly of liposomes, Dendrimersomes, and Polymersomes with amphiphilic Janus dendrimers conjugated to Mono-and Tris-Nitrilotriacetic Acid (NTA, TrisNTA) enhances protein ... 4 2022
Q Xiao, N Rivera-Martinez, CJ Raab, JG Bermudez, MC Good, ML Klein, ...
Giant 9, 100089

Bond-Dependent Thole Model for Polarizability and Spectroscopy 4 2019
M DelloStritto, ML Klein, E Borguet
The Journal of Physical Chemistry A 123 (25), 5378-5387

Exponential scaling of water exchange rates with ion interaction strength from the perspective of dynamic facilitation theory 4 2019
RC Remsing, ML Klein
The Journal of Physical Chemistry A 123 (5), 1077-1084

Improved delivery of the anticancer drug Taxol by worm-like PEG-PCL micelles rationalized by coarse grain molecular simulations 4 2012
SM Loverde, ML Klein, DE Discher
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 243

Protein Motion: Simulation 4 2009
I Samish, J Gu, ML Klein
Structural Bioinformatics 2, 907-936

Structure of the pore region of the nicotinic acetylcholine receptor ion channel: a molecular dynamics simulation study 4 2002
L Saiz, ML Klein
BIOPHYSICAL JOURNAL 82 (1), 560A-560A

- [Ab initio molecular dynamics simulations of molecular crystals](#) 4 1995
ME Tuckerman, T von Rosenvinge, ML Klein
MRS Online Proceedings Library (OPL) 408
- [Structural transitions in the heavily strained cyanide crystal \(KCl\) 0.25 \(KCN\) 0.75](#) 4 1989
LJ Lewis, ML Klein
Physical Review B 40 (11), 7904
- [Molecular dynamics calculation of the infrared and Raman spectra of ice IX in the translational mode region](#) 4 1987
ST John, ML Klein
Chemical physics letters 142 (3-4), 175-180
- [Elastic constants of solid ammonia](#) 4 1985
RW Impey, ML Klein
The Journal of chemical physics 83 (10), 5346-5347
- [JA Venables edtd.: RARE GAS SOLIDS vol. II](#) 4 1977
ML Klein
Academic Press
- [Brillouin spectroscopy and elastic constants](#) 4 1977
BP Stoicheff, ML Klein, JA Venables
Rare gas solids 2, 979-1020
- [Difference between zero-and first-sound propagation in solid Kr](#) 4 1975
VV Goldman, ML Klein
Physical Review B 12 (10), 4577
- [Lattice Dynamics of He 3 and He 4 at High Pressures](#) 4 1970
GG Chell, VV Goldman, ML Klein, GK Horton
Physical Review B 2 (2), 560
- [On the elastic constants of polycrystalline argon](#) 4 1968
C Feldman, ML Klein
The Philosophical Magazine: A Journal of Theoretical Experimental and ...
- [Dissolving salt is not equivalent to applying a pressure on water](#) 3 2022
C Zhang, S Yue, AZ Panagiotopoulos, ML Klein, X Wu
Nature communications 13 (1), 1-6
- [Discovery of Novel Small-Molecule Inhibitors of SARS-CoV-2 Main Protease as Potential Leads for COVID-19 Treatment](#) 3 2021
A Manandhar, V Srinivasulu, M Hamad, H Tarazi, H Omar, DJ Colussi, ...
Journal of Chemical Information and Modeling 61 (9), 4745-4757
- [From examining the relationship between \(corona\) viral adhesins and galectins to glyco-perspectives](#) 3 2021
ML Klein, A Romero, H Kaltner, V Percec, HJ Gabius

Biophysical journal 120 (6), 1031-1039

Aggregation of poly(*p*-phenylene terephthalamide) chains: Emergence of fiber defects 3 2019

S Mogurampelly, CM MacDermaid, S Percec, ML Klein, G Fiorin
Physical Review Materials 3 (1), 015602

Frontiers of macromolecular and supramolecular science symposia 3 2018

ML Klein, V Percec
Polymer Chemistry 9 (18), 2355-2358

Facially amphiphilic polyaryl and polyarylkynyl polymers and oligomers and uses thereof 3 2014

WF DeGrado, D Liu, GN Tew, ML Klein
US Patent 8,716,530

Effect of carboxylation on carbon nanotube aqueous dispersibility: A predictive coarse-grained molecular dynamics approach 3 2012

C Chiu, RH DeVane, ML Klein, W Shinoda, PB Moore, SO Nielsen
The Journal of Physical Chemistry C 116 (43), 23102-23106

I.; Thompson, ME 3 1998

AP Alivisatos, PF Barbara, AW Castleman, J Chang, DA Dixon, ML Klein, ...
Adv. Mater 10, 1297-1336

Physics of Cryocrystals 3 1997

ML Klein, AA Maradudin
AIP Press

Effect of physical factors on ultrasound attenuation and velocity in bone 3 1993

D Lin, W Xu, M Klein, T Einhorn, JJ Kaufman, RS Siffert
JOURNAL OF BONE AND MINERAL RESEARCH 8, S319-S319

Intermolecular interactions and the nature of orientational ordering in the solid fullerenes C₆₀ and C₇₀ 3 1992

A Cheng, ML Klein, M Parrinello, M Sprik
Philosophical Transactions of the Royal Society of London. Series A ...

Structural Organization in Self-Assembled Monolayers 3 1991

J Hautman, ML Klein
Computer Simulation in Materials Science, 395-405

Molecular dynamics study of the alloy (N₂) 67 (Ar) 29 3 1985

S Nosé, ML Klein
Canadian Journal of Physics 63 (10), 1270-1273

Dynamics of Impure Rare-Gas Crystals 3 1984

SS Cohen, ML Klein
Inert Gases, 87-144

- Vibrational amplitudes of xenon overlayers physisorbed on the graphite basal plane** 3 1983
SF O'Shea, Y Ozaki, ML Klein
Chemical Physics Letters 94 (4), 355-358
- Dynamical structure factor of metallic sodium at high temperatures** 3 1979
G Jacucci, ML Klein
Solid State Communications 32 (6), 437-440
- Herausgeber. Rare Gas Solids** 3 1976
ML Klein, JA Venables
Academic Press, London
- Quantum second virial coefficient of a two-dimensional Lennard-Jones gas** 3 1965
ML Klein
Molecular Physics 10 (1), 87-89
- SPICA Force Field for Proteins and Peptides** 2 2022
S Kawamoto, H Liu, Y Miyazaki, S Seo, M Dixit, R DeVane, ...
Journal of Chemical Theory and Computation 18 (5), 3204-3217
- Chain-end modification: A starting point for controlling polymer crystal nucleation** 2 2021
KW Hall, S Percec, W Shinoda, ML Klein
Macromolecules 54 (4), 1599-1610
- In-Silico Electrophysiology: On the Activation of Voltage-Gated Ion Channels using Molecular Dynamics Simulations** 2 2016
M Tarek, L Delemotte, M Kasimova, ML Klein, V Carnevale
Biophysical Journal 110 (3), 107a
- Density functional theory-based treatments of metal binding sites in metalloenzymes: Challenges and opportunities** 2 2014
M Alfonso-Prieto, ML Klein
Metalloproteins: structure, function and interactions
- Polymersomes for drug delivery through target-controlled release** 2 2005
F Ahmed, G Srinivas, ML Klein, T Minko, DE Discher
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 230, U1233-U1234
- Coarse-grain molecular dynamics study of peptide nanotube insertion in lipid bilayers.** 2 2005
B Ensing, SO Nielsen, PB Moore, ML Klein
Abstracts of Papers of the American Chemical Society 229, U771-U771
- New approach to efficiently explore the free energy surface, trace the reaction pathways and converge the free energy barriers** 2 2005
B Ensing, A Laio, M Parrinello, ML Klein
Abstracts of Papers of the American Chemical Society 229, 083-COMP

- Coarse-grain molecular dynamics study of nanotube insertion in lipid bilayers.** 2 2004
B Ensing, SO Nielsen, PB Moore, ML Klein
Abstracts of Papers of the American Chemical Society 228, U221-U221
- Coarse-grain molecular dynamics simulations of hydrophile cation translocation across a lipid bilayer.** 2 2004
G Srinivas, CF Lopez, ML Klein
Abstracts of Papers of the American Chemical Society 228, U221-U221
- Cover Picture: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. Int. Ed. 9/2004)** 2 2004
D Liu, S Choi, B Chen, RJ Doerksen, DJ Clements, JD Winkler, ML Klein, ...
Angewandte Chemie International Edition 43 (9), 1033-1033
- Ice Ih-Ice XI phase transition: A quantum mechanical study** 2 2004
JL Kuo, ML Klein, SJ Singer, L Ojamäe
AMER CHEMICAL SOC
- Exploration of the structural features defining ion channel conduction** 2 1999
GR Dieckmann, JD Lear, QF Zhong, ML Klein, WF DeGrado, KA Sharp
BIOPHYSICAL JOURNAL 76 (1), A200-A200
- Influenza A M2 ion channel-A molecular dynamics study** 2 1998
QF Zhong, T Husslein, DM News, P Pattnaik, ML Klein
BIOPHYSICAL JOURNAL 74 (2), A233-A233
- Molecular dynamics investigation of the lamellar liquid-crystal D-phase in the octylammonium chloride/water system** 2 1996
DJ Tobias, ML Klein
Molecular Simulation 16 (4-6), 219-228
- Molecular Dynamics Studies of Microscopic Wetting Phenomena/Molekulardynamische Untersuchungen von Benetzungerscheinungen** 2 1993
W Mar, J Hautman, ML Klein
Tenside Surfactants Detergents 30 (4), 252-255
- Use of an all-atom semiflexible model in molecular dynamic simulation of long chain paraffins** 2 1991
JP Ryckaert, IR Mc Donald, ML Klein, RJ Roe
Computer Simulation of Polymers
- COMPUTER-SIMULATIONS IN CONDENSED PHASES-PREFACE** 2 1989
ML Klein, PJ Rossky
CHEMICAL PHYSICS 129 (2), U163-U163
- SOLVATION-GENERAL DISCUSSION** 2 1988
D Chandler, H FRIEDMAN, J HYNES, P SUPPAN, B CONWAY, ...

Faraday Discussions 85

- [La périnatologie en Europe: des leçons à tirer](#) 2 1987
M Klein
Canadian Family Physician 33, 545
- [The rotator phase of solid caesium cyanide](#) 2 1982
ML Klein, Y Ozaki, IR McDonald
Journal of Physics C: Solid State Physics 15 (24), 4993
- [Orientational ordering of quadrupoles on a simple cubic lattice](#) 2 1980
SF O'Shea, ML Klein
Solid State Communications 33 (2), 179-181
- [Computer Modeling of Matter](#) 2 1978
ML Klein
ACS Symposium Series No. 86, 94
- [Monte Carlo calculations of the elastic constants of xenon](#) 2 1977
ML Klein, SF O'Shea
Chemical Physics Letters 48 (3), 555-559
- [Computer Simulation of Dynamical Properties of Bulk Solids](#) 2 1974
LJ Lewis, ML Klein
Dynamical Properties of Solids, 383-492
- [Isotope effects in physical adsorption and the interaction between argon atoms and graphitized carbon blacks](#) 2 1965
G Casanova, M De Paz, MG Dondi, ML Klein, G Scoles
Discussions of the Faraday Society 40, 188-194
- [Potential Pro-Inflammatory Effect of Vitamin E Analogs through Mitigation of Tetrahydrocannabinol \(THC\) Binding to the Cannabinoid 2 Receptor](#) 1 2022
A Manandhar, MH Haron, SA Ross, ML Klein, KM Elokely
International journal of molecular sciences 23 (8), 4291
- [Shear response in crystalline models of poly \(p-phenylene terephthalamide\)](#) 1 2021
G Fiorin, MJ DelloStritto, S Percec, ML Klein
Molecular Physics 119 (19-20), e1948122
- [Does Proton Conduction in the Voltage-Gated Proton Channel hHV1 Involve Grotthuss Hopping via Acidic Residues?](#) 1 2017
L Delemotte, S Van Keulen, U Roethlisberger, E Gianti, V Carnevale, ...
Biophysical Journal 112 (3), 163a-164a
- [Thermal Ripples in Model Molybdenum Disulfide Monolayers](#) 1 2017
RC Remsing, UV Waghmare, ML Klein
Zeitschrift für anorganische und allgemeine Chemie 643 (2), 152-154
- [Correction for Thomaston et al., High-resolution structures of the M2](#) 1 2016

- [channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction.](#)
JL Thomaston, M Alfonso-Prieto, RA Woldeyes, JS Fraser, ML Klein, ...
Proceedings of the National Academy of Sciences of the United States of ...
- [Advanced Modeling of the Human Skin Barrier](#) 1 2015
CM MacDermaid, RH DeVane, ML Klein, G Fiorin
Biophysical Journal 108 (2), 243a
- [Understanding the molecular determinants of capsaicin mode of action](#) 1 2015
KM Elokely, E Palovack, L Delemotte, V Carnevale, ML Klein
Biophysical Journal 108 (2), 57a
- [Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory.](#) 1 2015
J Hénin, MA Kasimova, A Kolocouris, ML Klein, S Khalid, MJ Lemieux, ...
J. Membr. Biol. 248
- [Development of a coarse-grained model for the surfactant family of linear alkylbenzene sulfonates](#) 1 2011
X He, W Shinoda, R Devane, O Guvench, KL Anderson, AD MacKerell, ...
Biophysical Journal 100 (3), 147a
- [Embedded Cholesterol in the Nicotinic Acetylcholine Receptor Embedded Cholesterol in the Nicotinic Acetylcholine Receptor](#) 1 2009
G Brannigan, J Henin, R Law, R Eckenhoff, ML Klein
BIOPHYSICAL JOURNAL 96 (3), 168A-168A
- [Embedded Cholesterol in the Nicotinic Acetylcholine Receptor](#) 1 2009
G Brannigan, J Henin, R Law, R Eckenhoff, ML Klein
Biophysical Journal 96 (3), 168a
- [Peptide hydrolysis in thermolysin: Reactant structure and reaction mechanism studied with classical and QM/MM molecular dynamics](#) 1 2006
G Lamoureux, J Blumberger, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 256-256
- [Breaking down endolysosomal barriers for drug delivery with degradable polymersomes](#) 1 2005
F Ahmed, G Srinivas, A Brannan, ML Klein, FS Bates, DE Discher
05AIChE: 2005 AIChE Annual Meeting and Fall Showcase
- [Coarse grain models for the simulation of soft matter and biomaterials: The challenge of bridging length and time scales to probe nature's designs](#) 1 2005
ML Klein
AIChE Annual Meeting
- [Cover Picture: The Design and Evaluation of Heparin-Binding Foldamers \(Angew. Chem. Int. Ed. 41/2005\)](#) 1 2005
S Choi, DJ Clements, V Pophristic, I Ivanov, S Vemparala, JS Bennett, ...

Angewandte Chemie International Edition 44 (41), 6599-6599

[Interaction of inhalational anesthetic halothane with membrane protein: A molecular dynamics study.](#) 1 2004

S Vemparala, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U181-U182

[The distribution of general anesthetics in membranes: Computer simulation of halothane in DPPC](#) 1 1999

D Scharf, L Koubi, M Tarek, M Klein

Anesthesiology 91 (3 A), U359-U359

[The vacuum structure of a synthetic four-alpha-helix bundle which binds halothane](#) 1 1999

LA Davies, ML Klein, D Scharf

BIOPHYSICAL JOURNAL 76 (1), A383-A383

[Computer simulation study of synthetic 4-helix bundle that binds halothane](#) 1 1998

AB Woska, ML Klein, D Scharf

Toxicology letters 100, 377-385

[Formation and stability of the LS3 synthetic ion channel.](#) 1 1998

QF Zhong, PB Moore, ML Klein

Abstracts of Papers of the American Chemical Society 215, U565-U565

[Ion channels: A challenge for computer simulations](#) 1 1998

Q Zhong, T Husslein, ML Klein

Classical and Quantum Dynamics in Condensed Phase Simulations, 463-486

[Pulsed terahertz study and spectral analysis of a simple solution; HCl in CCl4](#) 1 1997

BN Flanders, P Moore, R Cheville, M Klein, D Grischkowsky, NF Scherer

Quantum Electronics and Laser Science Conference, QWD46

[Modelling and simulation of solids](#) 1 1996

M Stoneham, ML Klein

Current Opinion in Solid State & Materials Science 6 (1), 817-819

[John Adair Barker.](#) 1 1996

D Henderson, M Klein

Physics Today 49 (8), 80-81

[Molecular dynamics simulation of lipid bilayers](#) 1 1996

DJ Tobias, K Tu, ML Klein

CONFERENCE PROCEEDINGS-ITALIAN PHYSICAL SOCIETY 49, 325-344

[Melting of Aromatic Compounds: Molecular Dynamics Simulations](#) 1 1995

PWC Kung, JT Books, CM Freeman, SM Levine, B Vessali, JM Newsam, ...

MRS Online Proceedings Library (OPL) 408

- Simple Models of Intermolecular Potential for the Condensed Phases of C₆₀** 1 1993
Z Gamba, ML Klein
Condensed Matter Theories, 535-542
- Molecular-dynamics study of lattice vibrations in the mixed crystal K 0.5 Rb 0.5 Cl** 1 1991
ER Cowley, ML Klein
Physical Review B 44 (10), 5000
- Simulations of Microscopic Wetting Phenomena on Self-Assembled Monolayers.** 1 1991
J Hautman, ML Klein
MRS Online Proceedings Library (OPL) 237
- Molecular-Dynamics Simulation Of Ordered And Rotator Phases Of Paraffins** 1 1989
JP Ryckaert, IR Mcdonald, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 198, 246-POLY
- Computer simulation of collective modes in solids** 1 1978
ML Klein
- Correction to a previous pseudopotential calculation of the elastic constants of sodium** 1 1976
SS Cohen, ML Klein, MS Duesbery, R Taylor
Journal of Physics F: Metal Physics 6 (10), L271
- On the temperature dependence of the cubic anharmonic contribution to the Helmholtz free energy of a simple crystal model** 1 1969
ML Klein, VV Goldman, GK Horton
Journal of Physics C: Solid State Physics 2 (9), 1542
- Superhydrophilicity of α -alumina surfaces results from tight binding of interfacial waters to specific aluminols** 2022
R Wang, Y Zou, RC Remsing, NO Ross, ML Klein, V Carnevale, ...
Journal of Colloid and Interface Science 628, 943-954
- Allosteric inhibitors of the main protease of SARS-CoV-2** 2022
SK Samrat, J Xu, X Xie, E Gianti, H Chen, J Zou, JG Pattis, K Elokely, ...
Antiviral research 205, 105381
- Structural insights into sodium chloride solutions from state-of-the-art neural network potentials** 2022
C Zhang, S Yue, A Panagiotopoulos, M Klein, X Wu
Bulletin of the American Physical Society
- Illuminating Stress and Failure in Polyethylene with a Neural Network Potential** 2022
M Dellostritto, S Percec, M Klein

Bulletin of the American Physical Society

[Superhydrophilicity of \[formula omitted\]-alumina surfaces results from tight binding of interfacial waters to specific aluminols](#) 2022

R Wang, Y Zou, RC Remsing, NO Ross, ML Klein, V Carnevale, ...

[Modeling the Ultrafast Electron Attachment Dynamics of Solvated Uracil](#) 2021

CS Anstoter, M DelloStritto, ML Klein, S Matsika

The Journal of Physical Chemistry A 125 (32), 6995-7003

[Regulation and drug modulation of a voltage-gated sodium channel: Pivotal role of the S4–S5 linker in activation and slow inactivation](#) 2021

J Xiao, V Bondarenko, Y Wang, A Suma, M Wells, Q Chen, T Tillman, ...

Proceedings of the National Academy of Sciences 118 (28), e2102285118

[The Early Stages of Polymer Crystallization: Nucleus-Induced Nucleation and Interfacial Structuring](#) 2021

K Hall, S Percec, W Shinoda, M Klein

APS March Meeting Abstracts 2021, M71. 125

[Modeling liquid water by climbing up Jacob's ladder in density functional theory facilitated by deep neural network](#) 2021

C Zhang, M Chen, L Zhang, M Klein, J Perdew, X Wu

APS March Meeting Abstracts 2021, L25. 002

[From examining the relationship between \(corona\) viral adhesins and mammalian galectins to glyco-perspectives](#) 2020

ML Klein, A Romero, H Kaltner, V Percec, HJ Gabius

Elsevier

[TRPA1 modulation by piperidine carboxamides suggests an evolutionarily conserved binding site and gating mechanism \(vol 116, pg 26008, 2019\)](#) 2020

T Chernov-Rogan, E Gianti, C Liu, E Villemure, AP Cridland, X Hu, ...

PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF ...

[Probing Heterogeneous Charge Distributions at the \$\alpha\$ -Al₂O₃ \(0001\)/H₂O Interface](#) 2020

SM Piontek, M DelloStritto, B Mandal, T Marshall, ML Klein, E Borguet

[Simulations at multiple scales reconcile lipid membrane structure with the barrier function of mammalian skin](#) 2019

G Fiorin, C MacDermaid, R Devane, M Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 258

[Designing biomacromolecular materials with tailored \(poly\) peptide conjugates](#) 2019

K Kiick, M Klein, K Elokely, E Gianti, V Carnevale

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 258

- Diffraction-like methodologies discover encoded biological recognition in bicomponent cell membrane mimics** 2019
M Young, C Rodriguez-Emmenegger, Q Xiao, NY Kostina, M Klein, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 258
- On the many roles played by lipids in the activation TRPV1, the noxious heat and capsaicin receptor** 2019
E Gianti, A Yazici, M Kasimova, T Rohacs, M Klein, V Carnevale
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 258
- Activation of TRPV1 by Lipids: Can Lipid Tails Bridge the Gap between the Vanilloid Binding Site and the Peripheral Cavities?** 2019
E Gianti, ML Klein, T Rohacs, V Carnevale
Biophysical Journal 116 (3), 536a
- Volume-Dependent Atomic Polarizabilities for Vibrational Spectroscopy** 2019
M Dellostritto, R Wang, M Klein, E Borguet
APS March Meeting Abstracts 2019, P16. 006
- Mechanism of water oxidation catalyzed by cobalt-intercalated layered MnO₂: confinement and intercalant local ordering** 2019
J Ning, J Furness, Y Zhang, A Thenuwara, R Remsing, M Klein, ...
APS March Meeting Abstracts 2019, B47. 001
- Bridging X-ray absorption spectra and nuclear quantum effects in the hydrogen bond network of liquid water** 2018
Z Sun, L Zheng, M Chen, M Klein, X Wu, F Paesani
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 256
- Crystals, liquid crystals, plastic crystals, & more...** 2018
M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 256
- Elucidating the hierarchical basis for supramolecular orientational memory** 2018
B Partridge, D Sahoo, M Peterca, E Aqad, M Imam, M Klein, V Percec
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 256
- X-ray Absorption Spectral Signature of Quantum Nuclei in Liquid Water** 2018
Z Sun, L Zheng, M Chen, ML Klein, X Wu
- Modifying layered manganese oxides for enhanced water oxidation: Turning a cheap, poor catalyst into a cheap, excellent catalyst** 2018
M Zdilla, D Strongin, E Borguet, M Klein, J Perdew, I McKendry, R Ding, ...
Abstracts of Papers of the American Chemical Society 255
- Molecular Insights into TRPV1 Polymodal Activation: Is Allosteric Coupling between the Toxin and the Vanilloid Binding Sites Mediated by Annular Lipids?** 2018
E Gianti, M Klein, T Rohács, V Carnevale

Biophysical Journal 114 (3), 396a

Why does hydronium diffuse faster than hydroxide in liquid water? 2018

M Chen, L Zheng, B Santra, HY Ko, RA DiStasio Jr, ML Klein, R Car, X Wu
arXiv preprint arXiv:1801.07841

Ab initio theory and modeling of water 2018

M Chen, HY Ko, R Remsing, M Calegari Andrade, B Santra, Z Sun, ...
APS March Meeting Abstracts 2018, P57. 002

Computational study of mechanical properties of poly-phenylene terephthalamide 2018

J Yu, G Fiorin, H Peng, M Klein, J Perdew
APS March Meeting Abstracts 2018, H43. 004

Effect of Structure and Functional on the SFG Spectrum at the Alumina-Water Interface 2018

M DelloStritto, S Piontek, E Borguet, M Klein
APS March Meeting Abstracts 2018, E17. 014

Self-assembly of Poly (p-phenylene terephthalamide) Nanofibrils: Emergence of Structural Defects 2018

S Mogurampally, G Fiorin, M Klein
APS March Meeting Abstracts 2018, Y53. 006

Tunable two-dimensional interfacial coupling in molecular heterostructures 2018

H Chakraborty, B Xu, VK Yadav, Z Zhang, ML Klein, S Ren
APS March Meeting Abstracts 2018, A17. 014

Molecular dynamics simulations of alkali halide adsorption to water-alumina interfaces 2017

R Wang, K Millan, R Remsing, S Piontek, A Tuladhar, L Magidson, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 254

Interlayer expanded layered manganese oxide for enhanced pseudocapacitive electrochemical energy storage 2017

A Thenuwara, N Attanayake, S Shumlas, R Remsing, M Klein, D Strongin
Abstracts of Papers of the American Chemical Society 254

Effect of the interlayer spacing and charge of 1T-MoS₂ on the electrocatalytic activity for the hydrogen evolution reaction 2017

N Attanayake, A Thenuwara, A Patra, Y Aulin, H Chakraborty, E Borguet, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 254

Ligand-and receptor-based virtual screening for inhibitors of the signal transducer and activator of transcription 5 (STAT5) 2017

E Gianti, G Fiorin, M Klein, R Zauhar
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 253

- Comparative analysis of the structural determinants of endogenous cannabinoids and activity of illicit drugs on cannabinoid receptors** 2017
V Yadav, K Elokely, M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 253
- Intercalation of metal ions into the interlayer region of layered manganese oxide for improved water oxidation electrocatalysis** 2017
D Strongin, A Thenuwara, S Shumlas, I McKendry, R Remsing, M Zdilla, ...
Abstracts of Papers of the American Chemical Society 253
- Why does hydronium diffuse much faster than hydroxide in liquid water?** 2017
M Chen, L Zheng, B Santra, HY Ho, R DiStasio Jr, M Klein, R Car, X Wu
APS March Meeting Abstracts 2017, A26. 007
- Dynamics of N-methylacetamide in methanol via ab initio molecular dynamics** 2017
VK Yadav, ML Klein
APS March Meeting Abstracts 2017, K26. 003
- Exploiting water density fluctuations in ion channel drug design** 2017
E Gianti, L Delemotte, M Klein, V Carnevale
Abstracts of Papers of the American Chemical Society 253
- Optimal decomposition of hydrogen-bonded water clusters for drug design** 2016
E Gianti, R Zauhar, M Klein, G Fiorin
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Enhanced water oxidation by nickel intercalated birnessite** 2016
A Thenuwara, E Cerkez, S Shumlas, N Attanayake, I McKendry, L Frazer, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Comparative analysis of the structural determinants of endogenous cannabinoids** 2016
V Yadav, K Elokely, M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Divergent synthesis of four generations of aliphatic polyamide dendrimers** 2016
Y Timsina, D Jishkariani, S Grama, C MacDermaid, S Gillani, M Divar, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Structural insight into agonist activity of cannabinoid receptor type-2 ligands using molecular dynamics simulation** 2016
V Yadav, K Elokely, M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Molecular structure of the human skin barrier and its response to external agents** 2016
C MacDermaid, M Klein, G Fiorin
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252

- Exploring the role of solvation in ion channel folding** 2016
D Granata, P Po, M Klein, C Deutsch, V Carnevale
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Divergent-convergent strategy for the synthesis of aliphatic polyamide dendrimers** 2016
S Grama, Y Timsina, D Jishkariani, C MacDermaid, S Gillani, M Divar, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Programming biological membrane mimics and their glycan with self-assembling Janus glycodendrimersomes** 2016
V Percec, Q Xiao, S Zhang, P Leowanawat, S Yadavalli, M Goulian, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Biomimicking membranes from Janus glycodendrimers reveal sugar-lectin recognition** 2016
Q Xiao, S Zhang, E Wang, S Sherman, RO Moussodia, M Peterca, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Lipid phase coexistence forms the basis of the permeability barrier of the outer skin layer** 2016
C MacDermaid, M Klein, G Fiorin
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 252
- Facially Amphiphilic Polymers and Oligomers and Uses Thereof** 2016
WF DeGrado, GN Tew, ML Klein, D Liu, J Yuan, S Choi
US Patent App. 14/958,709
- Accurate materials properties from an efficient density functional** 2016
R Remsing, J Sun, J Perdew, M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 251
- Skryabin, Philosophy and the Music of Desire** 2016
ML Klein
Music Analysis 35 (1), 110-118
- PNAS PLUS** 2016
Q Xiao, SS Yadavalli, S Zhang, SE Sherman, E Fiorin, L da Silva, ...
PNAS 113 (9), 2337-2340
- Modeling activation states in the voltage-gated proton channel 1 (Hv1) as a strategy for drug discovery** 2016
E Gianti, L Delemotte, M Klein, V Carnevale
Abstracts of Papers of the American Chemical Society 252
- 3 Density Functional Theory-Based Treatments of Metal-Binding Sites in Metalloenzymes** 2015
M Alfonso-Prieto, ML Klein
Metalloproteins: Theory, Calculations, and Experiments, 95

- Multiscale Simulations of Membranes** 2015
M Klein
APS March Meeting Abstracts 2015, D19. 005
- Dehydration of Multilamellar Fatty Acid Membranes: Towards a Computational Model of the Stratum Corneum** 2015
CM MacDermaid, RH Devane, ML Klein, G Fiorin
Biophysical Journal 108 (2), 243a
- Unveiling Potential Binding Sites in the Hv1 Four Helix Bundle** 2015
E Gianti, L Delemotte, V Carnevale, F Tombola, D Tobias, ML Klein
Biophysical Journal 108 (2), 424a-425a
- Molecular Determinants of Voltage Sensor Domain Activation** 2015
L Delemotte, V Carnevale, ML Klein, MA Kasimova, M Tarek
Biophysical Journal 108 (2), 427a
- Gating Pore Currents are Common Defects of Two Nav1.5 Mutations in Patients with Mixed Arrhythmias and Dilated Cardiomyopathy** 2015
A Moreau, P Gosselin-Badaroudine, L Delemotte, ML Klein, M Chahine
Biophysical Journal 108 (2), 572a
- Interaction of Ribonuclease III with the Regulatory Macrodomain Protein YmdB Analyzed by Docking Calculations and SPR Experiments** 2015
M Alfonso-Prieto, S Paudyal, SK Redhu, V Carnevale, ML Klein, ...
Biophysical Journal 108 (2), 225a
- Concentration Effect on the Hydrogen-Bond Strength between Small Molecules at the Oil/Water Interface: Application to Coarse-Grained Model Development** 2015
VK Yadav, C MacDermaid, G Fiorin, ML Klein
Biophysical Journal 108 (2), 243a
- Sequence Signature of Voltage Sensing Detected via Dimensionality Reduction Techniques** 2015
D Granata, M Marsili, ML Klein, V Carnevale
Biophysical Journal 108 (2), 426a
- Comparative Sequence Analysis Suggests a Unified Gating Mechanism for TRP Channels** 2015
V Carnevale, E Palovcak, L Delemotte, M Klein
Biophysical Journal 108 (2), 37a
- PIP2 Modifies the Free Energy of the Kv1.2 Voltage-Sensor Activation** 2015
MA Kasimova, L Delemotte, ML Klein, V Carnevale, M Tarek
Biophysical Journal 108 (2), 120a
- Flipping in the pore: Discovery of dual inhibitors that bind in different orientations to the wild-type versus the amantadine-resistant s31n mutant of** 2014

[the influenza a virus m2 ...](#)

W Degrado, Y Wu, B Canturk, H Jo, C Ma, E Gianti, ML Klein, LH Pinto, ...

[Proton release from the histidine-tetrad in the M2 channel of the influenza A virus](#)

2014

W Degrado, H Dong, G Fiorin, WF Degrado, ML Klein

[N-methylacetamide in the gravy of methanol: Ab initio molecular dynamics study](#)

2014

VK Yadav, A Bankura, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Deconstructing the pathways of ion conduction to describe the geometry of inhibition sites of the flu's proton channel](#)

2014

G Fiorin, E Gianti, M Alfonso-Prieto, V Carnevale, JL Thomaston, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Accurate prediction of electronic and structural properties of aqueous chloride and hydroxide ion from modern density functional theory](#)

2014

A Bankura, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Combining shape-based recognition and molecular simulation in drug discovery](#)

2014

E Gianti, RJ Zauhar, M Alfonso-Prieto, JL Thomaston, WF DeGrado, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Rational design of inhibitors targeting drug resistant mutants of the influenza A virus M2 proton channel](#)

2014

J Wang, Y Wu, B Canturk, H Jo, C Ma, G Fiorin, ML Klein, RA Lamb, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Solvation of cations in biological channels](#)

2014

V Carnevale, A Bankura, L Delemotte, L Stock, W Treptow, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Discovery of dual inhibitors targeting both WT and the S31N mutant of the influenza A virus M2 proton channel](#)

2014

J Wang, Y Wu, C Ma, B Canturk, H Jo, G Fiorin, ML Klein, RA Lamb, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[Water molecules work in concert to direct the traffic of protons in a viral membrane channel](#)

2014

M Alfonso-Prieto, G Fiorin, J Thomaston, V Carnevale, WF DeGrado, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 248

[The molecular mode of action of the active component of chili pepper](#)

2014

KM Elokely, E Palovcak, L Delemotte, V Carnevale, ML Klein

Planta Medica 80 (10), P12

- Systematic investigation of the electronic and structural properties of chloride ion in aqueous solution by advanced density functional** 2014
A Bankura, C Swartz, ML Klein, X Wu
APS March Meeting Abstracts 2014, Q3. 009
- Genomics-Aided Structural Modeling of an Antiparallel Homodimeric Fluoride Channel** 2014
EJ Palovcak, L Delemotte, ML Klein, V Carnevale
Biophysical Journal 106 (2), 148a
- Multi-Dimensional Free Energy Landscape of Voltage Sensor Domain Activation** 2014
L Delemotte, M Kasimova, V Carnevale, ML Klein, M Tarek
Biophysical Journal 106 (2), 233a
- Interaction of the Inward Rectifier Potassium Channel Kir 2.2 with Phosphatidylserine** 2014
MA Prieto, L Delemotte, ML Klein
Biophysical Journal 106 (2), 99a
- Role of Model Proteins on Membrane Fusion** 2014
HK Kashyap, ML Klein, G Fiorin
Biophysical Journal 106 (2), 504a
- Do Acidic Residues in the Tri-Asp Motif of the CNGA3 S2 Domain Form Required Pairings with Positive Residues of the S1-S4 Bundle? Evidence from Day-Blind Dogs and Insights from ...** 2014
N Tanaka, L Delemotte, ML Klein, AM Komáromy, JC Tanaka
Biophysical Journal 106 (2), 759a
- Exploring the Role of Pore Waters and Counterions in the Calcium Release-Activated Calcium Channel Conductance with Computation** 2014
H Dong, G Fiorin, ML Klein
Biophysical Journal 106 (2), 315a
- Characterizing Na⁺/K⁺ Permeation Rates through the Bacterial NavAb Sodium Channel** 2014
L Stock, V Carnevale, W Treptow, ML Klein
Biophysical Journal 106 (2), 131a-132a
- Networks of Coevolving Residues in Voltage Sensor Domains** 2014
V Carnevale, E Palovcak, L Delemotte, M Klein
Biophysical Journal 106 (2), 743a
- Reprint of: Neon interatomic potentials from scattering data and crystalline properties** 2013
JM Farrar, YT Lee, VV Goldman, ML Klein
Chemical Physics Letters 589, 14-16

- [Historical perspective on: Neon interatomic potentials from scattering data and crystalline properties \[Volume 19, Issue 3, 1 April 1973, Pages 359–362\]](#) 2013
JM Farrar, YT Lee, VV Goldman, ML Klein
Chemical Physics Letters 589, 12-13
- [Exploring histidine conformations in the M2 channel lumen of the influenza A virus at neutral pH via molecular simulations](#) 2013
W Degrado, H Dong, G Fiorin, WF Degrado, ML Klein
- [Gating of the calcium release-activated calcium channel: Insights from molecular simulations of the wild type and V174A mutant](#) 2013
H Dong, V Carnevale, G Florin, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 246
- [Probing the deprotonation mechanism of the His37 tetrad in the M2 channel from the influenza A virus via molecular simulation](#) 2013
H Dong, ML Klein, G Fiorin
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 245
- [Coarse-grained molecular dynamics of PEGylated assemblies](#) 2013
SM Loverde, W Shinoda, DE Discher, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 245
- [Investigating the Voltage Sensor Domains of Nav1. 4, its Structural and Functional Properties via Histidine Scanning Mutagenesis](#) 2013
P Gosselin-Badaroudine, L Delemotte, A Moreau, ML Klein, M Chahine
Biophysical Journal 104 (2), 133a
- [Binding of Isoflurane to a Bacterial Voltage-Gated Sodium Channel: Structure and Accessibility of Distinct Interaction Sites](#) 2013
SG Raju, V Carnevale, DN Lebard, AF Barber, ML Klein
Biophysical Journal 104 (2), 136a
- [PIP2-Mediated Gating of the Inward Rectifier Potassium Channel Kir2. 2](#) 2013
M Alfonso-Prieto, L Delemotte, ML Klein
Biophysical Journal 104 (2), 431a
- [Voltage Gated Cation Channels Activation: Towards an Ab-Initio Kinetic Model](#) 2013
L Delemotte, M Kasimova, M Tarek, W Treptow, V Carnevale, ML Klein
Biophysical Journal 104 (2), 279a
- [Volatile General Anesthetic Interactions with a Bacterial Sodium Channel](#) 2013
AF Barber, SG Raju, D Lebard, V Carnevale, ML Klein, M Covarrubias
Biophysical Journal 104 (2), 136a
- [Conduction and Selectivity of Ions through a Sodium Channel](#) 2013
L Stock, L Delemotte, V Carnevale, W Treptow, ML Klein

Biophysical Journal 104 (2), 173a

Structural Basis for Activation of Voltage-Gated Cation Channels

2013

C Amaral, V Carnevale, M Klein, W Treptow
Biophysical Journal 104 (2), 137a

Exploring Volatile General Anesthetic Binding to a Closed Membrane-Bound Bacterial

2013

SG Raju, AF Barber, DN LeBard, ML Klein, V Carnevale

MODES OF MOLECULAR SOLIDS AND LIQUIDS

2012

G Jacucci, ML Klein
Vibrational Spectroscopy of Molecular Liquids and Solids 56, 431

Center for Molecular Modeling and Department of Chemistry

2012

S BANDYOPADHYAY, M TAREK, ML KLEIN
New Approaches to Problems in Liquid State Theory: Inhomogeneities and Phase ...

Department of Chemistry University of Pennsylvania Philadelphia, Pennsylvania 19104-6323

2012

J HAUTMAN, ML KLEIN
Computer Simulation in Materials Science: Interatomic Potentials, Simulation ...

Molecular dynamics simulations of cell-penetrating homochiral cyclic peptides

2012

M Alfonso-Prieto, SM Loverde, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 244

Structure of water at charged surfaces: A molecular picture

2012

S Dewan, A Eftekhari-Bafrooei, V Carnevale, G Fiorin, ML Klein, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 244

Watching ions and water conduction through sodium channels

2012

W Treptow, L Stock, V Carnevale, M Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 244

QM and QMMM/MD investigation on the His37 configuration in the M2 proton channel

2012

H Dong, G Fiorin, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 244

Unraveling the binding of histidine kinase inhibitors by molecular dynamics simulations

2012

M Alfonso-Prieto, SM Loverde, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 244

Simulating the self-assembly of mixed surfactant micelles with graphics processing unit accelerated coarse-grained molecular dynamics

2012

DN LeBard, BG Levine, S Xiao, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 243

- Simulating ligand receptor binding at a membrane interface with graphics processing accelerated coarse-grained molecular dynamics** 2012
SM Loverde, DN Lebard, Z Ma, ML Klein, DE Discher
APS March Meeting Abstracts 2012, Y47. 002
- Mapping Water Density to Design New Blockers Against a Viral Proton Channel** 2012
G Fiorin, V Carnevale, J Wang, C Ma, T Wang, F Hu, R Lamb, L Pinto, ...
Biophysical Journal 102 (3), 682a
- Ion Binding Sites and Hydration in the Selectivity Filter of the Bacterial Sodium Channel Navab** 2012
V Carnevale, W Treptow, ML Klein
Biophysical Journal 102 (3), 603a
- On the function and modulation of the Kv1. 2 voltage-gated ion channel: Insights from large-scale all-atom molecular dynamics simulations.** 2011
L Delemotte, W Treptow, ML Klein, M Tarek
F1000Research 2
- Influence of solvation and interparticle interactions on the aggregation behavior of nanoparticles in membranes** 2011
U Ranatunga, A Jusufi, RH DeVane, W Shinoda, ML Klein, SO Nielsen
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 241
- Transmembrane Domain Packing in Cys-Loop Receptors: What Can we Learn from Prokaryotes?** 2011
G Brannigan, J Henin, R Eckenhoff, M Klein
Biophysical Journal 100 (3), 277a
- Association of Transmembrane Helices in Viral Fusion Peptides Suggests a Protein-Centric Mechanism of Membrane Fusion** 2011
G Fiorin, JE Donald, Y Zhang, V Carnevale, DR Slochower, F Gai, ...
Biophysical Journal 100 (3), 633a
- Dominant Site Involved in Inhibition of Targets by Anesthetics Suggested Through Novel Free Energy Perturbation Calculations** 2011
D LeBard, G Brannigan, J Henin, R Eckenhoff, M Klein
Biophysical Journal 100 (3), 195a
- Effect of sensor domain mutations on the properties of voltage-gated ion channels: molecular dynamics studies of the potassium channel (vol 99, pg L72, 2010)** 2011
L Delemotte, W Treptow, ML Klein, M Tarek
BIOPHYSICAL JOURNAL 100 (1), 269-269
- Quantitative Description of Electron Transfer Reactions** 2010
PHL Sit, A Migliore, ML Klein, N Marzari

Fuel Cell Science: Theory, Fundamentals, and Biocatalysis, 457-487

Effect of spherical fullerenes on pulmonary lipid monolayers: Molecular dynamics simulations 2010

SO Nielsen, C Chiu, PB Moore, R DeVane, ML Klein, W Shinoda
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 240

Viral fusogenic peptides form transmembrane helical bundles: Implications for the mechanism of fusion 2010

Y Zhang, J Donald, G Fiorin, V Carnevale, D Slochower, ML Klein, ...
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 240

Molecular simulation: Five decades and counting 2010

ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 240

Coarse grained molecular dynamics of biological and soft matter systems 2010

RH DeVane, W Shinoda, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 240

Charge sequestration and rectification of the M2 proton channel of influenza A 2010

BG Levine, G Fiorin, V Carnevale, WF DeGrado, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 239

DNA–nanotube hybrids: Small 1/2010 2010

RR Johnson, ATC Johnson, ML Klein
Small 6 (1)

COARSE GRAINED MODELS FOR PHENYL-BASED MOLECULES: APPLICATION TO FULLERENES 2010

C Chiu, R DeVane, ML Klein, W Shinoda, PB Moore, SO Nielsen
MOLECULAR DYNAMICS SIMULATIONS OF NANOSCALE INTERFACES: FROM SIMPLE LIQUIDS ...

Quantitative description of electron-transfer reactions from first-principles 2010

PHL Sit, A Migliore, ML Klein, N Marzari
Geochimica Et Cosmochimica Acta 74 (ARTICLE), A967-A967

Effect of magnesium ion concentration on the catalytic activity of ribonuclease H: Does a third metal bound at the active site modulate endonuclease catalysis? 2010

M Ho, M De Vivo, M Dal Peraro, ML Klein
Abstracts Of Papers Of The American Chemical Society 240 (CONF), 394-PHYS

Multiple Modes of Interaction between the Nicotinic Acetylcholine Receptor and Isoflurane Observed Through Long Time Simulations 2010

G Brannigan, D Lebard, J Henin, R Eckenhoff, ML Klein
Biophysical Journal 98 (3), 134a

- Curvature-driven Molecular Demixing in the Budding and Breakup of Mixed Component Worm-like Miscelles** 2010
LM Sharon, V Ortiz, RD Kamien, ML Klein, DE Discher
- Double gaps along Shaker S4 demonstrate omega currents at three different closed states** 2010
L DELEMOTTE, W TREPTOW, ML KLEIN, M TAREK
Biophysical journal 99 (11)
- Effects of Isoflurane Binding in the Pore of a Ligand-Gated Ion Channel** 2010
DN LeBard, G Brannigan, J Hénin, R Eckenhoff, ML Klein
Biophysical Journal 98 (3), 133a
- Calculation of the free energy of binding of DNA bases on a single-wall carbon nanotube** 2009
R Johnson, AT Johnson, M Klein
APS March Meeting Abstracts, B26. 003
- Collective variable-based calculations in NAMD** 2009
G Fiorin, J Henin, ML Klein
Biophysical Journal 96 (3), 406a-407a
- Wednesday, March 9, 2011 633a** 2009
G Fiorin, JE Donald, Y Zhang, V Carnevale, DR Slochower, F Gai, ...
Interaction 190, 199
- First Principles Molecular Dynamics Investigation of Bulk and Interfacial Aqueous Fluoride** 2008
M Ho, IW Kuo, ML Klein
Journal of Physical Chemistry A, vol. 113, no. 10, January 27, 2009, pp ...
- PRES 6-Physical chemistry is alive and well** 2008
ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 236
- COMP 128-Ab initio DFT plus Hubbard U study of nonheme iron-dioxygen intermediates in superoxide reductase** 2008
PHL Sit, A Migliore, MH Ho, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 236
- COMP 127-Ab Initio density-functional theory approach to evaluating electronic couplings in transition-metal systems: Application to the hexa-aquo Fe²⁺/³⁺ redox couple.** 2008
A Migliore, PHL Sit, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 236
- PMSE 171-Multiscale modeling efforts for biodegradable diblock copolymers** 2008
SM Loverde, V Ortiz, DE Discher, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 236

- COMP 188-Block copolymers fluid-fluid phase separation: A coarse grained molecular dynamics study.** 2008
DA Pantano, ML Klein, PB Moore
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 236
- PHYS 223-A half century journey through physical chemistry** 2008
ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 235
- PHYS 271-Aggregation and nanotube formation of cyclic peptides at an oil-water interface using coarse grained molecular dynamics** 2008
E Khurana, R DeVane, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 235
- Self assembly of natural and synthetic membranes using coarse grain models** 2008
ML Klein
APS March Meeting Abstracts, L7. 001
- Structure of a DNA-carbon nanotube hybrid using replica exchange molecular dynamics** 2008
R Johnson, AT Johnson, M Klein
APS March Meeting Abstracts, W29. 011
- OpenAtom--Ab initio molecular dynamics package** 2008
R Car, ME Tuckerman, GJ Martyna, N Nystrom, M Klein, J Torrellas, ...
New York Univ.(NYU), NY (United States)
- Unraveling the enzymatic mechanism of the protein farnesyltransferase: A QM/MM study** 2008
MH Ho, M De Vivo, M Dal Peraro, ML Klein
Abstracts Of Papers Of The American Chemical Society 236 (CONF), 258-COMP
- Multi-Scale Modelling Efforts for Diblock Copolymers** 2008
S Loverde, V Ortiz, DE Discher, M Klein
The 2008 Annual Meeting
- Nanoparticle Incorporation and Aggregation In Block Copolymer Worm-Like Micelles** 2008
DA Christian, K Rajagopal, G Srinivas, ML Klein, DE Discher
The 2008 Annual Meeting
- 3. Self-Assembling Peptide Nanotubes Dimers in polar and nonpolar solvents Reproduced with permission from: Self-Assembling Cyclic Peptides: Molecular Dynamics Studies of Dimers ...** 2008
SON Ektakhurana, B Ensing, ML Klein
Computational Studies of Natural and Synthetic Ion Channels 110, 58
- Nanoscale organization in room temperature ionic liquids: a coarse grained** 2007

[molecular dynamics simulation study](#)The HTML version of this article has been enhanced with colour images.

BL Bhargava, R Devane, ML Klein, S Balasubramanian

[COMP 357-Coarse grain models for self-assembling systems](#) 2007

ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[COMP 25-Two-metal associative catalysis: Phosphodiester cleavage in ribonuclease H](#) 2007

M De Vivo, M Dal Peraro, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[COLL 26-Coarse-grained molecular simulation of surfactant self-assembly](#) 2007

W Shinoda, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[COMP 121-Disruption of membranes by antimicrobial oligomers: An atomistic view](#) 2007

J Henin, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[COMP 258-Multi-terascale molecular modeling of biological systems](#) 2007

R DeVane, W Shinoda, J Henin, M Dal Peraro, A Kohlmeyer, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[COMP 384-Multiproperty parametrization of a coarse grained model for proteins](#) 2007

R DeVane, W Shinoda, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[PHYS 10-Molecular modeling of bacterial sensing machineries](#) 2007

C Soto, M Dal Peraro, P Carloni, WF DeGrado, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[PHYS 233-Blocking and resistance mechanism in M2 channel from influenza A virus explored by molecular dynamics](#) 2007

E Khurana, S Vemparala, M Dal Peraro, R De Vane, WF DeGrado, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 234

[Nothing amuses more harmlessly than computation](#) 2007

ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 233, 425-425

[Probing the Structure of DNA-Carbon Nanotube Hybrids with Molecular Dynamics Simulations](#) 2007

RR Johnson, AT Johnson, ML Klein

APS March Meeting Abstracts, H27. 009

- Simulate the aggregation of transmembrane proteins by coarse grain model** 2007
X He, SO Nielsen, ML Klein
BIOPHYSICAL JOURNAL, 223A-223A
- BIOL 66-Understanding and improving de novo design of proteins: New insights from molecular dynamics modeling** 2006
K Spiegel, M Dal Peraro, JR Calhoun, WF DeGrado, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 943-943
- Understanding self-assembling cyclic peptide nanotubes in lipid bilayer by molecular dynamics** 2006
E Khurana, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 225-225
- PHYS 393-Molecular dynamics and experimental studies on the stability of spectrin repeats** 2006
V Ortiz, CP Johnson, ML Klein, DE Discher
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232
- Molecular dynamics study of gemini surfactants at the air/water interface** 2006
E Khurana, SO Nielsen, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 227-227
- ORGN 42-Nucleophilic attack of hydroxide on formamide in aqueous solution: Mechanistic insights from ab initio metadynamics calculations** 2006
J Blumberger, B Ensing, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232
- Quorum-quenching proteins as therapeutic targets: Binding and reaction mechanism** 2006
K Spiegel, M De Vivo, M Dal Peraro, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 258-258
- Nucleotidyl transfer modulation by second shell ligands at the RNase H bimetal site** 2006
M De Vivo, M Dal Peraro, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 45-45
- Neurotransmitter transporters in lipid bilayers: A molecular dynamics study** 2006
DA Pantano, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 356-356
- Dinuclear catalytic strategy among metallo beta-lactamase superfamily** 2006
M Dal Peraro, P Carloni, A Vila, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 56-56
- INOR 909-Simulation of long-range electron transfer in proteins using a combined QM/MM-classical molecular dynamics approach** 2006
J Blumberger, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232

Efficiency of bimetal-aided phosphodiester bond cleavage in nucleotidyl transfer reactions 2006

M Dal Peraro, M De Vivo, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232, 222-222

INOR 911-Water mediated proton shuttles in enzymatic phosphoryl transfers: Phosphatase activity in soluble epoxide hydrolase 2006

M De Vivo, B Ensing, M Dal Peraro, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232

PHYS 36-A non-bonded description of metalloprotein sites in molecular dynamics simulations 2006

M Dal Peraro, K Spiegel, G Lamoureux, M De Vivo, WF DeGrado, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 232

PHYS 593-Diabatic free energy curves from vertical gap energies: An ab initio molecular dynamics approach 2006

J Blumberger, I Tavernelli, ML Klein, M Sprik

ABSTR PAP AM CHEM S 232, ?-?

Nanoparticle-surfactant composite self-assembly and surface patterning 2006

G Srinivas, DE Discher, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 231

Molecular Dynamics Simulations of DNA-Functionalized Carbon Nanotube Chemical Sensors 2006

R Johnson, M Klein, A Johnson

APS March Meeting Abstracts, N31. 006

Characterization of Rare Modification on Variant Human TNF Protein 2006

MD Zolodz, H Chung, ML Klein

54 th ASMS Conference Proceedings

Shuichi Nose 2006

Y Kataoka, ML Klein

Physics Today 59 (2), 67

Parameterization of novel anticancer drugs via a QM/MM force matching procedure and effect of drug-binding on DNA flexibility 2006

K Spiege, A Magistrato, P Maurer, P Ruggerone, P Carloni, ...

American Chemical Society 232, 252-252

MD (T, F) and Experimental Studies on the Thermomechanical Stability of Three-Helix Bundle Repeats 2006

V Ortiz, C Johnson, ML Klein, DE Discher

The 2006 Annual Meeting

- Soft Matter Systems Simulated by Molecular Methods** 2006
V Ortiz, ML Klein, DE Discher
The 2006 Annual Meeting
- Autobiography of Michael L. Klein** 2006
ML Klein
Journal of Physical Chemistry B 110 (8), 3454-3455
- Investigation of DNA Decorated Carbon Nanotube Chemical Sensors** 2006
M Chen, SM Khamis, RR Johnson, C Staii, ML Klein, JE Fischer, ...
MRS Online Proceedings Library (OPL) 963
- Effects of Polydispersity on the Stability of Aqueous Block Copolymer Assemblies** 2006
V Ortiz, ML Klein, DE Discher
The 2006 Annual Meeting
- Parallel molecular dynamics simulation in NPT ensemble and its application to general anesthesia** 2005
KJ Oh, ML Klein
Eighth International Conference on High-Performance Computing in Asia ...
- Multiscale Simulation Studies on Mechanisms of Poration for Hydrolytically Degradable Diblock Copolymer Membranes** 2005
V Ortiz, SO Nielsen, ML Klein, DE Discher
The 2005 Annual Meeting
- Titelbild: The Design and Evaluation of Heparin-Binding Foldamers (Angew. Chem. 41/2005)** 2005
S Choi, DJ Clements, V Pophristic, I Ivanov, S Vemparala, JS Bennett, ...
Angewandte Chemie 117 (41), 6757-6757
- Molecular dynamics simulation of open and close conformations of KirBac1.1 in explicit lipid bilayer: Structural changes and aromatic localization at lipid/water interface** 2005
S Vemparala, C Domene, ML Klein
- Computer simulation studies on mechanisms of poration for hydrolytically degradable diblock copolymer membranes** 2005
V Ortiz, SO Nielsen, ML Klein, DE Discher
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 230, U1315-U1316
- Molecular dynamics of zinc proteins with charge transfer represented by a minimal electronegativity equalization scheme** 2005
G Lamoureux, M Dal Peraro, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 230, U2881-U2882
- Water diffusion across nano-bio-assemblies of block copolymers: A coarsegrain simulation study** 2005

- G Srinivas, DE Discher, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 230, U1280-U1280
- Roles of Hinges and Linkers in Protein Extension** 2005
D Discher, N Bhasin, V Ortiz, MF Klein
Bulletin of the American Physical Society
- Topologies of protonated water clusters: A combined study by vibrational predissociation spectra and Monte Carlo simulations** 2005
JL Kuo, HC Chang, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U802-U803
- Forcefield parameterization of inhalational anesthetics, halothane and isoflurane: An ab initio study** 2005
S Vemparala, I Ivanov, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U787-U787
- Simulating polymersomes-A fruitful collaboration in rational coarse graining.** 2005
DE Discher, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U760-U760
- Peptide nanotube aggregation and pore forming in phospho-lipid membranes.** 2005
B Ensing, SO Nielsen, PB Moore, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U630-U630
- Characterization of non-biological antimicrobial polymers in aqueous solution and at water-lipid interfaces from all atom and coarse grained molecular dynamics.** 2005
I Ivanov, S Vemparala, V Pophristic, K Kuroda, WF DeGrado, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U771-U771
- Effect of ions on the dipole moment and electronic properties of water: Insight from initio molecular dynamics.** 2005
I Ivanov, M Dal Peraro, S Raugei, B Chen, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U745-U745
- Development and applications of an arylamide force field for molecular simulations.** 2005
V Pophristic, S Vemparala, I Ivanov, ML Klein, WF Degrado
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U807-U807
- Coarse-grain molecular dynamics simulations of nonionic surfactant self-organization at the solid-liquid interface.** 2005
G Srinivas, SO Nielsen, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U630-U630
- Self-assembly of peptide nanotubes by molecular dynamics study.** 2005
E Khurana, SO Nielsen, B Ensing, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U772-U772

- [Interactions of alcohol, anesthetic and aromatic ligands with LUSH, an odorant binding protein using molecular dynamics simulations](#) 2005
S Vemparala, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 229, U799-U799
- [Coarse grain models for the simulation of soft matter and biomaterials](#) 2005
M Klein
APS March Meeting Abstracts, CCP. 2005004
- [Nuclear quantum effects on the structure and energetics of \(H₂O\) 6H⁺](#) 2005
JL Kuo, DC Clary, ML Klein, JL Kuo, DC Clary, ML Klein
Royal Society of Chemistry
- [Ionic charge transfer effects in water, channels and enzymes](#) 2005
M Dal Peraro, G Lamoureux, I Ivanov, S Raugei, A Magistrato, P Carloni, ...
- [Interaction of arylamide polymers with heparin and lipid bilayers](#) 2005
S Vemparala, V Pophristic, I Ivanov, ML Klein
BIOPHYSICAL JOURNAL 88 (1), 235A-235A
- [Interaction of small anesthetic molecules with membranes and membrane proteins](#) 2005
L Saiz, ML Klein
BIOPHYSICAL JOURNAL 88 (1), 426A-426A
- [Insight into the last step in the catalytic cycle of arginase from ab initio molecular dynamics](#) 2005
I Ivanov, ML Klein
BIOPHYSICAL JOURNAL 88 (1), 402A-403A
- [Hydrogen bond topology and proton ordering phase transitions in ice](#) 2005
SJ Singer, CJ Knight, JL Kuo, TK Hirsch, L Ojamäe, ML Klein
AMER CHEMICAL SOC
- [Degradable polymersomes that create new pathways for anti-cancer drugs](#) 2005
F Ahmed, RI Pakunlu, G Srinivas, ML Klein, T Minko, DE Discher
05AIChE: 2005 AIChE Annual Meeting and Fall Showcase
- [Ab initio molecular dynamics simulation of redox reactions of transition metal ions in aqueous solution and proteins](#) 2005
J Blumberger, I Tavernelli, ML Klein, M Sprik
Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United ...
- [Gemini surfactants at the air/water interface: A molecular dynamics study.](#) 2004
E Khurana, SO Nielsen, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U284-U284
- [Structure of protonated water clusters: Finite temperature behavior and low-](#) 2004

energy topologies.

JL Kuo, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U260-U260

Reaction coordinates that describe alpha-helix and beta-sheet folding.

2004

B Ensing, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U188-U188

Fine tuning by second shell ligands and role of the Zn-His-Asp/Glu triad in Zn-metalloenzyme active sites.

2004

P Muni, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U882-U882

Coarse-grain molecular dynamics study of interactions between transmembrane nanotubes.

2004

SO Nielson, B Ensing, PB Moore, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U454-U454

Modeling aluminum chlorohydrate polymers.

2004

L Pophristic, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U797-U797

Dynamical and structural features of the Aeromonas proteolytica aminopeptidase active site with emphasis on the role of second shell ligands: Insights from a quantum/classical ...

2004

P Muni, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U240-U240

Proton transfer in the active site of arginase: Insight from ab initio molecular dynamics.

2004

I Ivanov, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U208-U208

Binding of alcohols and anesthetics in an odorant binding protein LUSH: A molecular dynamics study.

2004

S Vemparala, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U290-U290

Molecular dynamics study of heparin-arylamide binding in aqueous solution.

2004

V Pophristic, ML Klein, WF DeGrado

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U196-U196

Effect of second shell Zn-ligand substitution in the human carbonic anhydrase II active site: Role of the Zn-HIS119-GLU117 triad.

2004

P Muni, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U202-U202

Computer simulation studies of amphiphiles: The continuing challenge of bridging time and length scales.

2004

ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U234-U234

Ground state of small protonated water clusters.

2004

M Mella, DC Clary, ML Klein, JL Kuo, M Taylor

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 228, U222-U222

Structure of protonated water clusters: Finite temperature behavior.

2004

JL Kuo, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227, U314-U314

Novel conformationally-constrained 8-helical beta-peptides.

2004

RJ Doerksen, B Chen, J Yuan, JD Winkler, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227, U150-U150

Joint computational-experimental approach to effective and selective antimicrobial oligomers.

2004

RJ Doerksen, B Chen, DH Liu, WF DeGrado, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227, U912-U912

Monte Carlo calculations for nucleation phenomena.

2004

Jl Siepmann, B Chen, MJ McGrath, CJ Mundy, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 227, U1031-U1031

Experiments & Simulations of Pathway Shifts & T-dependent Forced Unfolding of 3-helix Proteins

2004

D Discher, R Law, M Klein

APS March Meeting Abstracts 2004, S9. 003

Titelbild: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. 9/2004)

2004

D Liu, S Choi, B Chen, RJ Doerksen, DJ Clements, JD Winkler, ML Klein, ...

Angewandte Chemie 116 (9), 1051-1051

The transmembrane domain of the nicotinic acetylcholine receptor ion channel: Insights from molecular dynamics simulations on synthetic peptide models.

2004

L Saiz, ML Klein

BIOPHYSICAL JOURNAL 86 (1), 543A-543A

Multi-repeat unfolding in steered molecular dynamics on spectrin family proteins

2004

V Ortiz, SO Nielsen, ML Klein, DE Discher

BIOPHYSICAL JOURNAL 86 (1), 413A-413A

Biophysical Theory and Modeling-Transmembrane Peptide-Induced Lipid Sorting and Mechanism of La-to-Inverted Phase Transition Using Coarse-Grain Molecular Dynamics.

2004

SO Nielsen, CF Lopez, I Ivanov, PB Moore, JC Shelley, ML Klein

Biophysical Journal 87 (4), 2107-2115

- Methods, systems, and computer program products for simulating biomembranes using coarse grain models** 2003
SO Nielsen, CF Lopez, PB Moore, ML Klein
- Novel conformationally-constrained-peptides characterized by ¹H NMR chemical shifts** Electronic supplementary information ESI available: experimental procedures and spectral data ... 2003
RJ Doerksen, B Chen, J Yuan, JD Winkler, ML Klein
- Self-assembly, static and dynamic properties of polymer vesicles: A coarse grain molecular dynamics simulation study.** 2003
G Srinivas, JC Shelley, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U288-U288
- Role of second sphere ZN (2+) ligands in *Aeromonas proteolytica* aminopeptidase.** 2003
P Muni, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U442-U442
- Insights from a large scale ab-initio molecular dynamics study into dynamical and structural features of the *Aeromonas proteolytica* aminopeptidase active site.** 2003
P Muni, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U771-U771
- Mechanism of peptide-induced lamellar to inverted hexagonal phase transition in phospholipid systems using coarse grain molecular dynamics.** 2003
SO Nielsen, CF Lopez, PB Moore, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U276-U276
- Structural determinants of the catalytic activity of arginase: Insights from terascale quantum simulations of the arginase active** 2003
I Ivanov, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U770-U771
- Deprotonation of a Zn (II) coordinated water molecule in solution: Determining relative pKa's by constrained first principles molecular dynamics.** 2003
P Muni, I Ivanov, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U770-U770
- Hydrogen bonding structure and dynamics of water at the DMPC lipid bilayer surface from a molecular dynamics simulation.** 2003
CF Lopez, SO Nielsen, ML Klein, PB Moore
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U297-U297
- Self-assembly, static and dynamic properties of diblock copolymer vesicles: A coarse-grain molecular dynamics simulation study.** 2003
ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U397-U397

Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics methods. 2003

L Ivanov, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 226, U173-U173

Short Wavelength Collective Dynamics in Phospholipid Bilayers 2003

SH Chen, ML Klein, M Tarek, DJ Tobias

Physical Review Letters 87 (23)

Computer simulation studies of soft materials: the continuing challenge of bridging length and time scales 2003

ML Klein

APS March Meeting Abstracts 2003, X10. 003

Self-Organization of "Spherical"Supramolecular Dendrimers: A New Perspective from Molecular Dynamics Simulation 2003

EG Kim, ML Klein

APS March Meeting Abstracts 2003, B17. 015

Large scale density functional investigation of arginase-A binuclear manganese metalloenzyme. 2003

I Ivanov, ML Klein

Abstracts of Papers of the American Chemical Society 225, U517-U517

De novo design and synthesis of antimicrobial oligo-amino acid-salicylamide. 2003

DH Liu, J Yuan, B Chen, RJ Doerksen, S Choi, ML Klein, JD Winkler, ...

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U231-U231

Relative pKas from first principles molecular dynamics: The case of histidine deprotonation 2003

L Ivanov, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U787-U787

De novo design and synthesis of non-hemolytic biomimetic antimicrobial polymers. 2003

DH Liu, RJ Doerksen, B Chen, D Clements, ML Klein, WF DeGrado

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U184-U184

Accurate energetics for in-plane versus out-of-plane phenol, thiophenol, anisole, and thioanisole 2003

RJ Doerksen, B Chen, WF DeGrado, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U787-U787

Molecular Simulation of Nucleation Phenomena 2003

JI Siepmann, B Chen, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U788-U789

- Designed intramolecular hydrogen bonds stabilizing antimicrobial amphiphilic polymers.** 2003
RJ Doerksen, B Chen, DH Liu, WF DeGrado, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 225, U598-U598
- Molecular dynamics investigation on the distribution of volatile anesthetics in biomembranes** 2003
M Pickholz, K Oh, ML Klein
APS March Meeting Abstracts 2003, N17. 003
- A model for the nicotinic acetylcholine receptor ion channel: structure of the transmembrane M2 segments as a pentameric assembly in a lipid bilayer** 2003
L Saiz, ML Klein
APS March Meeting Abstracts 2003, B10. 005
- Effect of the pore region of a transmembrane ion-channel on the physical properties of a simple membrane** 2003
L Saiz, S Bandyopadhyay, ML Klein
BIOPHYSICAL JOURNAL 84 (2), 382A-382A
- Ab initio molecular dynamics study of the E2 and Sn2 reaction between X-+ CH3CH2Y** 2003
B Ensing, FL Gervasio, A Laio, M Parrinello, ML Klein
Abstracts of papers 226, U303-U303
- Bridged binuclear metal motif: Events preceding and following substrate binding in *Aeromonas Proteolytica* Aminopeptidase.** 2002
P Muni, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 224, U646-U647
- Computational design of biomimetic materials.** 2002
B Chen, RJ Doerksen, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 224, U510-U510
- Simulating liquid/vapor interfaces.** 2002
B Chen, JI Siepmann, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 223, U429-U429
- Molecular dynamics simulation of aggregates of A beta 16-22 peptide of beta-amyloid in water.** 2002
KJ Oh, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 223, C29-C29
- Ab initio study of aqueous NaOH solution.** 2002
B Chen, I Ivanov, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 223, C80-C80
- Aggregation-volume-bias monte carlo simulations of nucleation phenomena.** 2002
B Chen, JI Siepmann, KJ Oh, ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 223, U505-U505

Molecular Dynamics Simulation of Knot Dynamics in Polyethylene Melts 2002
EG Kim, ML Klein
APS March Meeting Abstracts, S10. 010

Structure and dynamics of the pore region of the nicotinic acetylcholine receptor ion channel: A molecular dynamics simulation study 2002
L Saiz, ML Klein
APS March Meeting Abstracts, J32. 007

Study of the structural and dynamical properties of a biomimetic compound of diiron proteins via ab initio and hybrid molecular dynamics simulations 2002
A Magistrato, U Rothlisberger, ML Klein
Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States ...

Computer simulations in condensed phases 2002
ML Klein, PJ Riossky
Chemical physics (ISSN 1873-4421 129 (2)

Study of the structural and dynamical properties of a biomimetic compound of diiron proteins via ab initio and hybrid (QM/MM) molecular dynamics simulations 2002
A Magistrato, U Rothlisberger, ML Klein
Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States ...

Soft matter: Colloids, foams and surface solutions-Self-assembly of a phospholipid Langmuir monolayer using coarse-grained molecular dynamics simulations 2002
CF Lopez, SO Nielsen, PB Moore, JC Shelley, ML Klein
Journal of Physics-Condensed Matter 14 (40), 9431-9444

Exploration in Accurate Atomistic, Coarse Grain and Mesoscopic Simulations of Structured Solutions 2002
JC Shelley, MY Shelley, BC Reeder, RA Crawford, BD Laidig, ...
Multiscale Modeling, Simulation and Visualization and Their Potential for ...

Biophysical Theory and Modeling-Molecular Dynamics Investigation of Membrane-Bound Bundles of the Channel-Forming Transmembrane Domain of Viral Protein U from the Human ... 2002
CF Lopez, M Montal, JK Blasie, ML Klein, PB Moore
Biophysical Journal 83 (3), 1259-1267

Center for Molecular Modeling and Department of Chemistry University of Pennsylvania, Philadelphia, PA 19104-6323 2001
Q ZHONG, T HUSSLEIN, ML KLEIN
New Horizons of Computational Science: Proceedings of the International ...

Molecular dynamics simulation studies of water in pores and cavities. 2001

- D Yarne, GJ Martyna, ME Tuckerman, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 221, U236-U236
- Molecular dynamics simulation studies of surfactant systems.** 2001
R Allen, S Bandyopadhyay, JC Shelley, MY Shelley, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 221, U309-U309
- Ab initio molecular dynamics study of topological defects in polymers** 2001
ML Klein, AM Saitta
APS March Meeting Abstracts, N19. 001
- Effect of unsaturations on the physical properties of a model membrane with the highly polyunsaturated docosahexaenoic fatty acid** 2001
L Saiz, ML Klein
APS March Meeting Abstracts, S21. 002
- Structure of the pore forming region of the nicotinic acetylcholine receptor ion channel** 2001
L Saiz, ML Klein
APS March Meeting Abstracts, Z21. 013
- The formation of a β -Peptide/DPC-micelle complex studied by MD simulations** 2001
I Antes, ML Klein
Poster book of the 1st Gordon Research Conference in Bioinformatics
- Structure of a model membrane with the highly polyunsaturated docosahexaenoic fatty acid** 2001
L Saiz, ML Klein
BIOPHYSICAL JOURNAL 80 (1), 521A-521A
- Comparing non-immobilizer to anesthetic distribution in a model membrane** 2001
D Scharf, L Koubi, M Tarek, S Bandyopdhyayi, ML Klein
BIOPHYSICAL JOURNAL 80 (1), 503A-503A
- Interdisciplinary Physics: Biological Physics, Quantum Information, etc.- Short Wavelength Collective Dynamics in Phospholipid Bilayers: A Molecular Dynamics Study** 2001
M Tarek, DJ Tobias, SH Chen, ML Klein
Physical Review Letters 87 (23), 238101-238101
- Molecular Dynamics Simulation of Ion Channels** 2001
Q Zhong, T Husslein, ML Klein
New Horizons of Computational Science, 169-181
- Molecular dynamics studies of membranes and membrane proteins.** 2000
ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 220, U162-U162

- Molecular dynamics studies of solvation.** 2000
ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 219, U289-U289
- Ab initio molecular dynamics study of topological defects in polyethylene strands** 2000
AM Saitta, ML Klein
APS March Meeting Abstracts, S36. 192
- Molecular dynamics simulations of (L38M-A alpha (2))(2) a four-helix bundle that specifically binds halothane** 2000
D Scharf, LA Davis, JS Johansson, ML Klein
ANESTHESIA AND ANALGESIA 90 (2)
- Low concentration of a non-anesthetic modify properties of a model bilayer** 2000
D Scharf, LA Davies, QF Zhong, JS Johansson, ML Klein
BIOPHYSICAL JOURNAL 78 (1), 186A-186A
- Properties halothane binding cavity in proteins** 2000
QF Zhong, LA Davies, RG Eckenhoff, ML Klein, D Scharf
BIOPHYSICAL JOURNAL 78 (1), 331A-331A
- Molecular dynamics simulations of two synthetic four-helix bundles that bind halothane** 1999
S Daphna, LA Davies, JS Johansson, ML Klein
ANESTHESIOLOGY 91 (3 A), U349-U349
- Molecular Dynamics Simulations of Two Synthetic Four-Helix Bundles That Bind Halothane** 1999
S Davies, JS Johansson, ML Klein
ANESTHESIOLOGY-PHILADELPHIA THEN HAGERSTOWN- 91 (3A), A751-A751
- The distribution of volatile general anesthetics in a model membrane** 1999
L Koubi, ML Klein, D Scharf
BIOPHYSICAL JOURNAL 76 (1), A139-A139
- Molecular dynamics simulations of heme group orientation and structure in a vectorially-oriented cytochrome c monolayer** 1999
CE Nordgren, AM Edwards, DJ Tobias, ML Klein, JK Blasie
BIOPHYSICAL JOURNAL 76 (1), A153-A153
- Polymers, Biopolymers, and Complex Systems-Polyethylene under tensile load: Strain energy storage and breaking of linear and knotted alkanes probed by first-principles molecular ...** 1999
AM Saitta, ML Klein
Journal of Chemical Physics 111 (20), 9434-9440
- Atomistic computer simulation studies of surfactant systems** 1999
S Bandyopadhyay, M Tarek, ML Klein

New Approaches to Problems in Liquid State Theory, 347-358

Effects of halothane on the structure of a hydrated DPPC bilayer 1998

D Scharf, KC Tu, M Tarek, ML Klein
ANESTHESIOLOGY 89 (3 A), U382-U382

Ab-initio path integral molecular dynamics of water wires 1998

ML Klein, HS Mei, ME Tuckerman, D Sagnella
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 215, U272-U272

A computer simulation to determine the structural and physical properties of a synthetic 4-alpha-helix bundle. 1998

AB Woska, BR Gibney, PL Dutton, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 215, U565-U565

The structure and dynamic properties of a synthetic 4-alpha-helix bundle. 1998

AB Woska, BR Gibney, JJ Skalicky, JA Wand, PL Dutton, ML Klein
BIOPHYSICAL JOURNAL 74 (2), A331-A331

The Nature of Titanylphthalocyanine Y-form Crystals in Photoreceptors 1998

O Okada, ML Klein
NIP & Digital Fabrication Conference 1998 (2), 512-515

Biophysical Theory and Modeling-Effects of anesthetics on the structure of a phospholipid bilayer: Molecular dynamics investigation of halothane in the hydrated liquid crystal ... 1998

K Tu, M Tarek, ML Klein, D Schaff
Biophysical Journal-Paper Edition 75 (5), 2123-2134

Gas Phase Dynamics and Structure: Spectroscopy, Molecular Interactions, Scattering, and Photochemistry-An ab initio path integral molecular dynamics study of double proton ... 1998

S Miura, ME Tuckerman, ML Klein
Journal of Chemical Physics 109 (13), 5290-5299

The structure of the surfactant-water interface for sodium octanoate micelles: A molecular dynamics study using polarizable models. 1997

JC Shelley, M Sprik, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 214, 46-COLL

Molecular dynamics studies of the electrostatics of micellar interfaces using a polarizable model. 1997

JC Shelley, M Sprik, ML Klein
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 214, 92-COMP

Potential functions for simulation of biological molecules-Foreword 1997

M Klein, M Marchi, J Smith
JOURNAL DE CHIMIE PHYSIQUE ET DE PHYSICO-CHIMIE BIOLOGIQUE 94 (7-8), R1-R1

Determination of conformational disorder in the fluid phase lipid bilayers by 1997

molecular dynamics simulation.

WJ Sun, KC Tu, DJ Tobias, ML Klein, HL Strauss, RG Snyder

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 213, 98-PHYS

Ab initio studies of acid solutions

1997

ML Klein

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 213, 190-PHYS

Computer Simulations of Membrane Protein Interactions

1997

ML Klein

APS March Meeting Abstracts, K7. 01

Potential functions for simulation of biomolecular systems Introduction

1997

ML Klein, M Marchi, JC Smith

Journal de Chimie Physique et de Physico-Chimie Biologique 7 (94), 1305-1312

A Phenomenological Model of the LS2 Ion Channel

1997

Q Zhong, DM Newns, ML Klein

MRS Online Proceedings Library (OPL) 489

Crystal hydrates of HCl studied using full ab initio path integral molecular dynamics

1996

ME Tuckerman, T vonRosenvinge, ML Klein, GJ Martyna

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 212, 269-PHYS

Molecular dynamics studies of lipid bilayers

1996

ML Klein, KC Tu, D Tobias

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 212, 258-PHYS

Electrostatic effects on ion conduction in designed helical bundle ion channels

1996

JD Lear, ML Klein, WF DeGrado, DM Newns, Q Zhong, J Schneider

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 212, 15-PHYS

AB-INITIO MOLECULAR-DYNAMICS SIMULATIONS OF HCL IN WATER

1995

K LAASONEN, ML KLEIN

Abstracts of papers of the American Chemical Society 210, 115-PHYS

MOLECULAR-DYNAMICS SIMULATIONS OF PHOSPHOLIPID-BILAYERS

1995

K TU, DJ TOBIAS, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 210, 151-PHYS

MOLECULAR-DYNAMICS SIMULATION OF SURFACTANT SYSTEMS AT THE AIR-WATER-INTERFACE

1995

M TAREK, DJ TOBIAS, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 210, 175-COLL

CONFORMATIONAL AND ORIENTATIONAL DISORDER IN SOLID POLYTETRAFLUOROETHYLENE

1995

M SPRIK, U ROTH LISBERGER, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 209, 375-PHYS

[Intermolecular motion in solid C \[sub 70\]: A molecular dynamics simulation study](#) 1994

M Sprik, ML Klein

Journal of Physical Chemistry;(United States) 98 (37)

MONTE-CARLO CALCULATIONS FOR ORGANIC MONOLAYERS 1994

JI SIEPMANN, ML KLEIN, IR MCDONALD

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 208, 50-COMP

[MOLECULAR-DYNAMICS SIMULATIONS OF PHOSPHOLIPID CRYSTALS, AND GEL AND LIQUID-CRYSTAL PHASE BILAYERS](#) 1994

DJ TOBIAS, KC TU, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 208, 49-COMP

[MOLECULAR-DYNAMICS SIMULATIONS OF C14TAB MONOLAYERS AT THE AIR-WATER-INTERFACE](#) 1994

M TAREK, DJ TOBIAS, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 208, 98-COMP

[MOLECULAR-DYNAMICS STUDIES OF ORGANIC THIN-FILMS](#) 1994

U ROTLISBERGER, W MAR, ML KLEIN

ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 207, 80-PHYS

[Philadelphia, Pennsylvania 19104-6323](#) 1994

J Hautman, ML Klein

Theoretical and Computational Approaches to Interface Phenomena, 149

[Domains and Superlattices in Self-Assembled Monolayers of Long-Chain Molecules](#) 1994

J Hautman, ML Klein

Theoretical and Computational Approaches to Interface Phenomena, 149-159

[Simulation of Self-Assembled Monolayers: Microscopic Structure of Amino Alkylthiols](#) 1994

U Röthlisberger, ML Klein, M Sprik

Computational Approaches in Supramolecular Chemistry, 399-409

[Electronic Spectra of a Lithium Impurity in Clusters, the Bulk Liquid, and Solid *para*- Hydrogen](#) 1994

D Scharf, GG Martyna, ML Klein

Reaction Dynamics in Clusters and Condensed Phases, 153-168

[Molecular dynamics studies of solid C {sub 60} and C {sub 70}](#) 1993

ML Klein, A Cheng

American Chemical Society, Washington, DC (United States)

MOLECULAR-DYNAMICS SIMULATIONS OF LANGMUIR MONOLAYERS WITH FULL ATOMIC DETAIL 1993

- JP BAREMAN, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 205, 208-COLL
- A MOLECULAR-DYNAMICS STUDY OF SAM-PHASE-DIAGRAM AND LOW-TEMPERATURE STRUCTURE** 1993
W MAR, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 205, 45-COLL
- Molecular dynamics studies of solid C₆₀ and C₇₀** 1993
ML Klein, A Cheng
205th ACS national meeting
- Intermolecular Interactions and the Nature of Orientational Ordering in the Solid Fullerenes C₆₀ and C₇₀: Discussion** 1992
M Lal, ML Klein
Philosophical Transactions of the Royal Society of London Series A 341 (1661 ...
- NOVEL QUANTUM EFFECTS IN PARA-HYDROGEN CLUSTERS-MELTING AND SUPERFLUIDITY** 1992
D SCHARF, GJ MARTYNA, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 204, 65-PHYS
- ISOTOPE EFFECT ON THE MELTING OF PARA-HYDROGEN CLUSTERS** 1992
D SCHARF, GJ MARTYNA, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 203, 279-PHYS
- QUANTUM SIMULATION STUDIES OF BIPOLARONS IN AMMONIA** 1992
Z DENG, GJ MARTYNA, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 203, 280-PHYS
- A MOLECULAR-DYNAMICS STUDY OF NEWTON BLACK FILMS** 1992
ML KLEIN, Z GAMBA, J HAUTMAN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 203, 325-PHYS
- Computer Simulation of Micelles in Aqueous Solution** 1992
ML Klein
Structure and Dynamics of Strongly Interacting Colloids and Supramolecular ...
- The electronic states of metal-ammonia clusters and solution** 1991
GJ Martyna, ML KLEIN
Le Journal de Physique IV 1 (C5), C5-103-C5-113
- Department of Chemistry University of Pennsylvania** 1991
J HAUTMAN, ML KLEIN
Computer Simulation in Materials Science: Interatomic Potentials, Simulation ...
- NUCLEAR-MAGNETIC-RESONANCE MEASUREMENT OF MASS-TRANSFER IN MOLECULAR-SIEVE CRYSTALLITES-DISCUSSION** 1991
J WALTON, CRA CATLOW, GB SUFFRITTI, P DEMONTIS, ML KLEIN, ...
JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS 87 (13), 1997-2010

- INTERFACIAL STRUCTURE FOR A COMPATIBLE POLYMER BLEND FOR SHORT AND INTERMEDIATE ANNEALING TIMES-DISCUSSION** 1991
RM LYDENBELL, LV WOODCOCK, JHR CLARKE, DJ TILDESLEY, ...
JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS 87 (13), 2063-2071
- ALKALI-METAL ATOMS IN XENON CLUSTERS** 1990
GJ MARTYNA, C CHENG, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 200, 95-PHYS
- Ultrafast rotational dynamics of electronically excited aniline molecules from ultraviolet femtosecond fluorescence anisotropies** 1990
MA Pereira, PE Share, MJ Sarisky, JC Shelley, ML Klein, ...
International Conference on Ultrafast Phenomena, MD5
- COMPUTER-SIMULATION OF QUANTUM ADIABATIC DYNAMICS BY MEANS OF A CLASSICAL SEPARATION OF TIME SCALES** 1989
M SPRIK, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 198, 32-PHYS
- MOLECULAR-DYNAMICS STUDIES OF LANGMUIR-BLODGETT FILMS** 1989
JP BAREMAN, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 197, 23-PHYS
- MOLECULAR-DYNAMICS STUDIES OF MICELLES IN AQUEOUS-SOLUTION** 1989
K WATANABE, ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 197, 29-PHYS
- Molecular Dynamics for Systems Under High Pressure** 1989
ML Klein, P Demontis
Simple Molecular Systems at Very High Density 186, 441
- CHARACTERIZATION OF A LANGMUIR—BLODGETT MONOLAYER USING MOLECULAR DYNAMICS CALCULATIONS** 1988
JPB Gianni CARDINI, ML KLEIN
CHEMICAL PHYSICS LETTERS 22, 1988
- SOLVATION-GENERAL DISCUSSION** 1988
HL FRIEDMAN, MH ABRAHAM, Y MARCUS, J ENGBERTS, ...
FARADAY DISCUSSIONS 85, 147-172
- SOLVATION-GENERAL DISCUSSION** 1988
M SYMONS, S TOMODA, T CLARK, M KLEIN, B ODINTSOV, ...
FARADAY DISCUSSIONS 85
- Morrison, James Alexander-Obituary** 1988
M KLEIN, S OSHEA, R WEIR, MA WHITE
Canadian Journal of Chemistry-Revue Canadienne De Chimie

- Diabatic Electron-Ion Recombination in a Polar Solvent** 1988
ML Klein, M Sprik
Chemical Reactivity in Liquids, 175-186
- A SYMPOSIUM ON INTERACTION-INDUCED SPECTRA IN DENSE FLUIDS AND DISORDERED SOLIDS, 10TH AND 11TH DECEMBER 1986-GENERAL DISCUSSION** 1987
M ZOPPI, AD BUCKINGHAM, T KEYES, IM DESCHEPPER, RA HUIJTS, ...
JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS II 83, 1921-1937
- The Rahman Festschrift** 1987
B Berne, D Chandler, M Klein
The Journal of Physical Chemistry 91 (19), 4865-4865
- ELECTION SOLVATION IN POLAR-SOLVENTS** 1986
M KLEIN, RW IMPEY, M SPRIK
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 191, 230-PHYS
- Computer simulation of molecular crystals** 1985
ML Klein, RW Impey
Journal de chimie physique 82, 111-115
- COMPUTER-SIMULATION STUDY OF MUONIUM IN WATER** 1984
ML KLEIN, M SPRIK, B DERAEDT
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 187 (APR), 67-PHYS
- Argon and Its Companions** 1984
ML Klein
Inert Gases, 1-4
- The disordered solid phases of potassium cyanide** 1983
IR McDonald, DG Bounds, ML Klein
Journal of Physics C: Solid State Physics 16 (17), 3217
- THE DIFFUSION OF LITHIUM IONS IN LITHIUM-SULFATE** 1983
ML KLEIN
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 185 (MAR), 49-PHYS
- COMPUTER-SIMULATION STUDIES OF PHYSISORBED OVERLAYERS** 1983
ML KLEIN, SF OSHEA
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 185 (MAR), 15-COLL
- Intermolecular potentials and condensed state properties** 1980
ML Klein
Molecular physics and quantum chemistry: into the 80's
- Rotation-Translation Coupling in Collective Modes of Molecular Solids and Liquids** 1980
G Jacucci, ML Klein

Vibrational Spectroscopy of Molecular Liquids and Solids, 431-441

Computer Simulation of Bulk Properties of Alkali Metals 1976

SS Cohen, ML Klein, MS Duesbery, R Taylor
Computer Simulation for Materials Applications. Nuclear Metallurgy. 20

THERMODYNAMIC PROPERTIES OF METALLIC SODIUM AT 293 DEGREESK AND 361 DEGREESK 1975

SS COHEN, ML KLEIN
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 20 (1), 103-103

RADIAL DISTRIBUTION FUNCTION OF LIQUID-SODIUM 1972

RD MURPHY, ML KLEIN
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 17 (1), 93-&

COMMENTS ON CLAIMED DIFFERENCE BETWEEN THERMAL AND ELASTIC DEBYE TEMPERATURES OF COPPER NEAR 0 DEGREES K 1972

ML KLEIN, DL MARTIN
PHYSICS LETTERS A, 430-&

Phonon energies and lifetimes in solid argon near 0 K 1970

VV Goldman, GK Horton, TH Keil, ML Klein
Journal of Physics C: Solid State Physics 3 (12), 2516

LATTICE DYNAMICS OF SOLID HCP H2 AND D2 1970

ML KLEIN, TR KOEHLER
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 15 (3), 277-&

ANHARMONIC CONTRIBUTIONS TO HELMHOLTZ FREE ENERGY OF AN FCC CRYSTAL 1968

JL FELDMAN, GK HORTON, ML KLEIN
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 13 (4), 689-&

THERMAL PROPERTIES OF SOLID AR KR AND XE 1968

GK HORTON, ML KLEIN, JL FELDMAN
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY 13 (4), 689-&

Isotope Separation in Physical Adsorption 1967

G Casanova, MG Dondi, G Scoles, ML Klein
Fundamentals of Gas-Surface Interactions, 258-270

GENERAL DISCUSSION ON INTERMOLECULAR FORCES 1965

IJ ZUCKER, ML KLEIN, JA BARKER, OK RICE, THK BARRON, ...
Discussions of the Faraday Society, 117-+

HIGH TEMPERATURE ADSORPTION AND INTERACTIONS BETWEEN ADSORBED MOLECULES 1965

DH EVERETT, JD JOHNSON, ML KLEIN
ANALES DE LA REAL SOCIEDAD ESPANOLA DE FISICA Y QUIMICA SERIA B-QUIMICA, 73-&

