

## BIODATA

**Name:** Narayanasami Sathyamurthy

**Born:** July 10, 1951

**Position:**

Honorary Professor, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru  
Chief Editor, Resonance – Journal of Science Education, Indian Academy of Sciences, Bengaluru  
Honorary Director, Centre for Cooperation in Science and Technology among Developing Societies (CCSTDS), Chennai

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[nsathyamurthy@gmail.com](mailto:nsathyamurthy@gmail.com)

**Academic Qualifications:**

B.Sc. Annamalai University, Annamalainagar 1970  
M.Sc. Annamalai University, Annamalainagar 1972  
Ph.D. Oklahoma State University, Stillwater OK USA 1975

**Positions Held:**

**Post-doctoral Fellow**, University of Toronto, Toronto Canada 1975-78  
**Assistant Professor**, University of Toronto, Toronto Canada 1977-78  
**Lecturer**, Indian Institute of Technology Kanpur, Kanpur 1978-80  
**Asst. Professor**, Indian Institute of Technology Kanpur, Kanpur 1980  
**Professor**, Indian Institute of Technology Kanpur, Kanpur 1985 – 2016  
**Institute Chair Professor**, Indian Institute of Technology Kanpur, Kanpur 2007 – 2016  
**Director**, Indian Institute of Science Education and Research (IISER) Mohali (June 2007 – September 2017)  
**Visiting Professor**, University of Rome, Rome, Italy, May-June 2000  
**Head**, Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 1998-2001  
**Convener**, Multi-Disciplinary Initiative in Biological Sciences and Bio-engineering, IIT Kanpur 2001-2002  
**Dean of Faculty Affairs**, Indian Institute of Technology Kanpur, Kanpur 2002-2004  
**Member** (Senate Nominee), **Board of Governors**, IIT Kanpur 1997-99

**Member, Council**, Indian Academy of Sciences, Bangalore, 2001-2006  
**Chairman**, National Scientific Committee, International Chemistry Olympiad, Mumbai, 2001  
**Founder President**, Association of Chemistry Teachers, 2001-2004.  
**Vice-President** (International Affairs), Indian National Science Academy, New Delhi 2010-12  
**Member, Scientific Advisory Committee to the Cabinet, Government of India**, 2013-2018  
**President, Chemical Research Society of India**, April 2017-March 2020

#### **Awards and Honors:**

**Young Scientist Medal**, Indian National Science Academy, New Delhi 1980  
**Young Associate**, Indian Academy of Sciences, Bangalore 1983  
**Alexander-von-Humboldt Fellow**, Max-Planck-Institut f. Strömungsforschung, Göttingen, Germany 1986-87  
**INSA Research Fellow**, Indian National Science Academy, New Delhi 1989-91  
**Rev. Yedanapalli Memorial Award**, Indian Chemical Society 1989  
**S.S. Bhatnagar Prize** in Chemical Sciences, Council of Scientific & Industrial Research, New Delhi 1990  
**Fellow**, Indian Academy of Sciences, Bangalore 1990  
**Fellow**, Indian National Science Academy, New Delhi 1992  
**Honorary Professor**, S. N. Bose National Center for Basic Sciences, Calcutta 1995-98  
**Sir C.V. Raman Award**, Hari Om Ashram Trust, University Grants Commission, New Delhi 1997  
**FICCI Award**, New Delhi 2001  
**Silver Medal**, Chemical Research Society of India, Bangalore 2001  
**Honorary Professor**, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore 2000-2002; 2007 - 2019  
**Professor Navneetha Rao Best Teacher Award**, Andhra Pradesh Academy of Sciences, Hyderabad 2003  
**Fellow**, The World Academy of Sciences, Trieste, Italy 2005  
**J. C. Bose National Fellow**, Department of Science and Technology, New Delhi, 2006-2016  
**Institute Fellow**, IIT Kanpur, 2013  
**SASTRA-CNR Rao Award for Chemistry and Material Science 2016**, Sastra University, Thanjavur, Tamilnadu  
**Sir C V Raman Medal**, Indian National Science Academy, New Delhi, 2016

#### **Ph.D. Theses Guided:**

I. NoorBatcha 1982  
Tomi Joseph 1983  
Sukarma Thareja 1985  
K. Raghavan 1986  
V. Mohan 1986  
N. Balakrishnan 1993  
Sanjay Kumar 1993  
C. Kalyanaraman 1994  
S. Mahapatra 1996

N. Chakrabarti 1997  
Shruti Maheshwary 2000  
B. Maiti 2001  
Aditya Narayan Panda 2004  
U. Lourderaj 2004  
Kousik Giri 2007  
Ashwani Kumar Tiwari 2007  
C. N. Ramachandran 2007  
Brijesh Kumar Mishra 2008  
Pradeep Kumar 2012  
Sujitha Kolakkandy 2012  
Saurabh Srivastava 2013  
Moumita Majumder 2013

**Edited: Reaction Dynamics: Recent Advances**, Narosa (New Delhi) and Springer-Verlag (Berlin) 1991

**Edited, along with R Bandyopadhyay:** Institution Building: The Story of IISERs, Indian Academy of Sciences, Bengaluru, 2018

**Chief Editor**, Resonance – Journal of Science Education, Jan. 2018-

**Member**, Editorial Board, Proceedings of Indian Academy of Sciences (Chemical Sciences) 1993 - 2000

**Member**, Editorial Board, IITK Series of Advanced Texts 1995-2000

**Member**, General Committee, International Conference on the Physics of Electronic and Atomic Collisions, 1993-96

**Editor**, Proceedings of Indian National Science Academy (Part A) 2000-2005

**Member**, Editorial Board, Indian Journal of Chemistry A 2001-2007

**Member**, Editorial Board, Indian Journal of Chemistry B 2005-2007

**Member**, Editorial Board, International Journal of Theoretical and Computational Chemistry, World Scientific, 2002-

**Member**, Editorial Board, International Reviews in Physical Chemistry, 2005-.

**Member**, Editorial Advisory Board, Journal of Physical Chemistry, 2007-2009

**Member**, Editorial Board, European Physical Journal D, 2010-2021

**Member**, Editorial Board, Current Science, 2015-

**Associate Editor**, Resonance – Journal of Science Education, Sep. 2017-Dec. 2017

**Sponsored Research Projects:**

Study of reactive and nonreactive collisions, DST 1980-84

Certain aspects of molecular reaction dynamics, DST 1984-87

Chemical Dynamics and Laser Spectroscopy, INDO-US project (collaborator: J.W. Gadzuk) 1986-91

Fractals, kinematics and complex formation, CSIR 1990-1993

Dynamics of molecular processes on surfaces, INDO-US Project (collaborator: J.W. Gadzuk) 1992-97

Ion-molecule reactions, CEC (Brussels) (collaborators: F.A. Gianturco and L.A. Zuelicke) 1993-97

Time-dependent quantum mechanical approach to reactive scattering and related processes, DST 1998-2002

Structure and stability of water clusters, protonated water clusters, water clusters in a constrained environment and gas hydrates and molecular solvation, CSIR 2003-2006

Optical and Electrical properties of doped fullerenes and carbon nanotubes, DMSRDE, Kanpur 2006-2009

Non-adiabatic processes, Indo-Portugal Project (Collaborator: A J C Varandas) 2007-2010

**Organized:**

Winter School on Molecular Reaction Dynamics January 1-14, 1984

The Second Winter School on Molecular Reaction Dynamics Dec. 27, 1987 - January 9, 1988

**Co-organized** with Professor P. Raghunathan:

Symposium on Magnetic Resonance, Instrumentation and Theoretical Chemistry, July 29-31, 1988

**Co-organized** with Professors B. M. Deb and S. Ramasesha

Discussion Meeting on Time-dependent quantum mechanics of many electron systems,  
JNCASR & IISc Bangalore, Jan. 9-12, 1996

**Co-organized** with Professor R. Ramaswamy

TC2K: Discussion Meeting on Theoretical Chemistry, IIT Kanpur Dec. 22-24, 2000

**Co-organized** with Professor T. K. Chandrashekar

Sixth CRSI National Symposium in Chemistry, IIT Kanpur Feb. 6-8, 2004

### **Invited Lectures**

#### **Conferences, Symposia and Winter/Summer Schools: India**

Annual Convention of Chemists, Kurukshetra September 24, 1978

Winter School on Theoretical Chemistry, Jadavpur University, Calcutta October 1981

Annual Convention of Chemists, Cuttack December 28, 1983

Symposium on Symmetry and Topology in Chemistry, Platinum Jubilee Celebrations of the Indian Chemical Society Jadavpur October 17, 1984

Annual Meeting of the Indian Council of Chemists, Gorakhpur January 1, 1985

DST/PAC workshop on Update in Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore January 13-14, 1985

National Conference on Theoretical Chemistry and Spectroscopy Jadavpur, Calcutta December 4-6, 1985

Winter School on Lasers in Chemical and Biological Sciences, I.I.T. Delhi December 18, 1987

Symposium on New Trends in Kinetics and Mechanism and Role of Trace Metal Ions, Univ. Rajasthan, Jaipur Feb. 20-23, 1988

Perspectives in Scientific Research, Bihar Council of Science and Technology, Patna March 26, 1988

Winter School on Statistical Mechanical Applications in Chemistry, I.I.T. Bombay December 22-24, 1988

National Symposium on Physical Organic Chemistry, Madurai Kamaraj University February 27-28, 1989

Symposium on Essential Role of Fundamental Scientific Research - jointly organized by the Indian National Science Academy and the Indian Academy of Sciences Bangalore Dec. 15, 1989

Symposium on Trends in Chemical Dynamics, Tata Institute of Fundamental Research, Bombay Dec. 17, 1989

Mid-Year Meeting, Indian Academy of Sciences, Bangalore July 27, 1990

DST Group Monitoring Workshop for Young Scientists, Shillong, August 27, 1990

Academy Discussions of Trends in Theoretical Chemistry, IIT Madras Sept. 30 - Oct. 1, 1990

8th National Workshop on Atomic and Molecular Physics, Univ. Hyderabad, December 6-11, 1990

Annual Convention of Chemists, Bodhgaya Univ., Gaya Dec. 27, 1990

All India Symposium on Structure, Activity and Dynamics: Advancing Frontiers, New Delhi June 3-4, 1991

DAE Symposium on Radiation and Photochemistry, BARC, Bombay Jan. 27-30, 1992

Discussion meeting on ultrafast processes in chemistry, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, Sep. 22-23, 1992

Academy meeting of theoretical chemistry, IIT Kharagpur, February 1993

S. N. Bose Centenary meeting, Calcutta, December 30, 1993 - January 2, 1994

Discussion meeting of "Computer simulations in materials research", Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, November 15-17, 1994

International Symposium on Spectra, Structure and Dynamics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta, November 28-30, 1994

Winter School on Chemical Applications of Statistical Mechanics, IIT Bombay, December 1994

Symposium on Density Functional Theory, Panjab University, Chandigarh, February 1995

Discussion meeting on quantum chemistry, Indian Institute of Science, Bangalore, July 26-27, 1995

Interdisciplinary Seminar, Indian National Science Academy, New Delhi, October 4, 1995

International Discussion Meeting on Time-Dependent Quantum Mechanics of Many Electron Systems, IISc Bangalore, Jan. 9-12, 1996

Discussion Meeting on Ion-Atom and Ion-Molecule Collision Phenomena, TIFR, Bombay January 29-31, 1996

National Seminar on Molecular Dynamics and Structure, IIT Madras April 5-6, 1996

Academy Discussion Meeting on Theoretical Chemistry, Mahatma Gandhi University, Kottayam, December 5-8, 1996

Workshop on "Recent Developments in Chaotic Dynamics", Bharatidasan University, Tiruchirapalli, December 9-13, 1996

National Seminar on Concepts in Chemistry, CMS College, Kottayam, February 10-13, 1997

Golden Jubilee Conference on Nonlinear Dynamics & Computational Physics, PRL, Ahmedabad, Nov. 18-22, 1997

XII International Conference on Computers in Chemical Research & Education, Univ. Poona, Pune, Jan. 5-9, 1998

Frontiers in Chemistry, Banaras Hindu University, Varanasi, Jan. 30-31, 1998

International Discussion Meeting on Intense Laser Fields and their Interaction with Matter, Goa, Feb. 17-19, 1998

International Discussion Meeting on Ultrafast Chemical Phenomena, JNCASR & IISc Bangalore, March 2-6, 1998

Frontiers in Inorganic Chemistry, IISc Bangalore, July, 1998

SERC School on "Atoms and Molecules in Intense Fields", PRL, Ahmedabad, February, 1999

Seminar on Ultrafast Processes in Biology, Chemistry and Physics, University of Madras, Chennai, March 11-13, 1999

National Seminar on Advances in Electron Transfer Processes, Madurai Kamaraj University, Madurai, July 15-16, 1999

International Conference on Chemistry and 36<sup>th</sup> Annual Convention of Chemists, Indian Chemical Society, Calcutta, Dec. 11-16, 1999

Indo-French Workshop on "Advances in the understanding of adsorption phenomena at solid/aqueous solution interfaces, TRDDC, Pune Feb. 12-15, 2001

Annual Meeting of the Chemical Research Society of India, National Chemical Laboratory, Pune, Feb. 1-3, 2002

Indo-Japan Joint Workshop on Frontiers of Molecular Science Developed by Advanced Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, Dec. 3-4, 2004

Fourth annual Convention of Chemistry Teachers, Science City, Ahmedabad, Nov. 2004

Theoretical Chemistry Symposium, BARC, Mumbai Dec. 9-12, 2004

XVth National Conference on Atomic and Molecular Physics, Physical Research laboratory, Ahmedabad, Dec. 20-23, 2004

Symposium on Structure and Dynamics, IIT Madras, Chennai April 22, 2005

Recent Advances in Nanoscience and Technology, Periyar University, Salem Sep. 29, 2005

Humboldt Kolleg, Banaras Hindu University, Varanasi November 28-30, 2005

Recent Trends in Fluorescence Spectroscopy and its Applications, Kumaun University, Nainital Dec. 1-3, 2005

National Symposium on Spectroscopy and its applications, Indian Association for the Cultivation of Science, Kolkata, January 18-20, 2006

Frontiers in Chemistry workshop, Department of Chemistry, Government Model Science College, Jabalpur, Sep. 15-16, 2006

IUPAC Discussion Meeting on Hydrogen Bond, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, Sep. 18, 2006

National Symposium on, "Advances in Chemistry and Environmental Impact", Department of Chemistry, North-Eastern Hill University, Shillong, November 2-3, 2006

7<sup>th</sup> Asian International Seminar on Atomic and Molecular Physics, Indian Institute of Technology Madras, Chennai, December 4-7, 2006

Theoretical Chemistry Symposium 2006, Bharathidasan University, Tiruchirappalli, Dec. 11-13, 2006

Indian National Science Congress, Annamalai University, Annamalainagar, Jan. 5-7, 2007

Discussion meeting on Spectroscopy and Dynamics of Molecules and Clusters, Corbett National Park, Uttaranchal, Feb. 23-25, 2007.

Reach2007, Timber Trails, Himachal Pradesh, March 7-10, 2007



Indo-German Symposium, Indian Institute of Chemical Technology, Hyderabad, September 2007

JNC Frontier Lectures, Gurunanak Dev University, Amritsar, October 24-26, 2007

Indo-German Symposium on Frontiers in Chemistry, IIT Kanpur Kanpur October 26-28, 2007

SERC School, NIPER, Mohali, June 30, 2008

International Conference and Humboldt Kolleg on Structural characterization and spectroscopy of materials relevant to nanotechnology, biomedical and geobiology, Banaras Hindu University, Varanasi, November 6-9, 2008

1<sup>st</sup> Inter IISER Chemistry Meet 2008, Indian Institute of Science Education and Research, Pune, December 22-23, 2008

Guru Nanak Dev University, Amritsar,

Punjab Science Congress, Punjab Agricultural University, Ludhiana, February 7, 2009

Discussion meeting on Crystal Engineering and Noncovalent Interactions: Contemporary themes and futuristic developments, Orange County, Coorg, February 22-25, 2009

India-Japan Workshop on Frontiers in Molecular Spectroscopy and Theory, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, March 7-9, 2009

Atoms and molecules in a confined environment, Foundation Day Lecture, Institute for Microbial Technology, Chandigarh, Sep. 26, 2009

UG Projects: curiosity Driven Science, IISER Bhopal, November 1, 2009

Curiosity driven science, CSIO, Chandigarh, November 30, 2009

Atomic and Molecular clusters: The story of a fruitful collaboration, Invited Lecture in the Symposium on Changing Paradigms in Theoretical and Computational Chemistry: From Atoms to Molecular Clusters, Department of Chemistry, University of Pune, Pune Dec. 18-20, 2009

Structural motifs and shapes of atomic and molecular clusters, Invited Lecture in the Symposium, "Of Molecules and Materials (A survey of recent concepts)", IISER Kolkata, Dec. 28-29, 2009

Stacking and spreading interaction in N-heteroaromatic systems, Invited Lecture in Inter IISER Meet in chemistry IISER Kolkata Dec. 30-31, 2009

Playing with the buckyball, Inaugural Address at the 3<sup>rd</sup> Winter School on Nanotechnology in drug delivery, National Institute of Pharmaceutical Education and Research, Mohali, February 7, 2010

Playing with the buckyball, SASE, Chandigarh, February 28, 2010

Playing with the buckyball, Department of Chemistry, Panjab University, Chandigarh, Sep. 13, 2010

IITK should be No. 1 again! REACH Symposium, IIT Kanpur, Kanpur Oct. 10-12, 2010

Playing with the buckyball, Theoretical Chemistry Symposium, IIT Kanpur, December 8-12, 2010

Curiosity driven science, INSPIRE camp, University of Kashmir, Srinagar, July 27, 2011

Playing with the buckyball, ATOMS2011, Indian Institute of Chemical Technology, Hyderabad, November 2, 2011

Chemistry: melting boundaries, International Year of Chemistry, National Chemical Laboratory, Pune, Nov. 24, 2011

Structural motifs and shapes of atomic and molecular clusters, International Conference on Innovations in Chemistry for Sustainable Development, Panjab University, Dec. 1, 2011

Structural motifs and shapes of atomic and molecular clusters, Celebration of Chemistry, IIT Kanpur, Dec. 4, 2011

A Mirchi Story: Curiosity Driven Science, INSPIRE Camp, University of Jammu, January 20, 2013

Pentagons and hexagons, Chennai Chemistry Conference 2013, CLRI, Chennai, Feb. 8, 2013

Pentagons and hexagons, New Frontiers in Chemistry, Punjabi University, Patiala, Feb. 16, 2013

Back to the basics: the case of diatomic anions, An international conference on electronic structure and dynamics of molecules and clusters, IACS, Kolkata, Feb. 17-20, 2013

From our garden back to the Gondwana land, Science City, Kapurthala, Feb. 28, 2013

Bowls, balls and sheets: five and six-fold symmetry, Punjab University, March 2, 2013

Pentagons and hexagons in bowls, balls, sheets and flowers, IISER Bhopal, March 15, 2013

Pentagons and hexagons in bowls, balls, sheets, tubes and flowers, Chemistry Department, Mahatma Gandhi University, Kottayam, March 25, 2013

Bowls, balls and sheets: five and six-fold symmetry, Symposium on Theoretical and Computational Chemistry Frontiers & Challenges, Bharathidasan University, Tiruchirapalli, June 14-15, 2013

From molecules to materials: challenges and opportunities in computational chemistry, International conference on “Computational and data intensive science”, CSIR Fourth Paradigm Institute, Bangalore, August 26-28, 2013

From atomic and molecular clusters to floral symmetry: the role of pentagons and hexagons, CF-2013: Chemical Frontiers, Goa, August 28-30, 2013

Indian Institutes of Science Education and Research (IISERs): An Indian Experiment in Science Education and Research, 2<sup>nd</sup> Summit of the South Asian Academy of Sciences, Indian National Science Academy, New Delhi, Sep. 25, 2013

Floral Symmetry, Complex Systems: From Physics to Biology, Jawaharlal Nehru University, New Delhi, Oct. 15-16, 2013

Symmetry and beauty of the floral world around us, Foundation Day Lecture, CSIO, Chandigarh, Oct. 30, 2013

Stacking and spreading interaction in molecular materials, International Conference on Interdisciplinary Areas with Chemical Sciences (ICIACS 2013), Panjab University, November 1, 2013

Back to the Basics: the Case of Diatomic Anions, 50<sup>th</sup> Annual Convention of Chemists, Department of Chemistry, Panjab University, Chandigarh, December 5, 2013

IISERs: An Indian Experiment in Science Education and Research, NIAS-DST training programme on “Policy for Science and Science for Policies”, Bangalore, December 19, 2013

IISERs: An Indian Experiment in Science Education and Research, SPSTI meeting on higher education in 21<sup>st</sup> century, Chandigarh, February 19, 2014

Symmetry in chemistry and the floral world, Spectroscopy and dynamics of molecules and clusters, Puri, Feb. 20-23, 2014

Structural motifs in chemistry and chemical biology, IV National Symposium on Advances in Chemical Sciences, GNDU, Amritsar, Feb. 27-28, 2014

Symmetry in chemistry and chemical biology, Academy Workshop on Recent Advances in Materials Science, Bharathidasan Institute of Technology, Anna University, Tiruchirapalli, March 8, 2014

Symmetry in chemistry and chemical biology, National Symposium on Chemistry, Aligarh Muslim University, Aligarh, March 22, 2014

Structural motifs in chemistry and chemical biology, National Conference on Mastering in Molecules and Materials (M<sup>3</sup>-2014), NIT Kurukshetra, October 16-17, 2014

Symmetry and pattern formation in flowers, International Symposium on Advances in Spectroscopy and Ultrafast Dynamics, IACS, Kolkata December 12-14, 2014

Back to the basics: the case of certain diatomics, Theoretical Chemistry Symposium, NCL Pune, Dec. 18-20, 2014

Probing molecules in real time and space and Structural motifs in chemistry, Academy Workshop on New Frontiers in Chemistry, Govt. Periyar Arts College, Cuddalore Jan. 29-30, 2015

Atoms and molecules in a confined environment, Academy Workshop on Current Trends in Chemistry, Varanasi Feb. 20, 2015

Noncovalent interactions and structural motifs in chemistry and chemical biology, JSPS-DST Asian Academic Seminar and School, IACS and IISER Kolkata, March 6-10, 2015

Symmetry and Pattern Formation in Flowers, Indian Academy of Sciences, Bangalore July 4, 2015

Symmetry and Pattern Formation in Flowers, INSPIRE meeting, Pandit Ravishankar Shukla University, Raipur July 27, 2015

Back to the basics: certain diatomics and triatomics, IISER Kolkata, January 28, 2016

Symmetry and Pattern Formation in Flowers, Sir J C Ghosh Memorial Lecture, Department of Chemistry, IIT Kharagpur, February 9, 2016

Symmetry and Pattern Formation in Flowers, Multani Mal Modi College, Patiala, February 19, 2016

Symmetry and Pattern Formation in Flowers, SASTRA University, Thanjavur, February 28, 2016

Structural motifs in chemistry and chemical biology, Anna University, Chennai, March 12, 2016

Non-adiabatic interactions and geometric phase, Recent Advances in Theoretical Chemistry, IISc, Bangalore, July 8-9, 2016

Institution building: the story of IISERs, Foundation Day Lecture, NISER, Bhubaneswar, September 6, 2016

Institution building: the story of IISERs, Biology Day Lecture, IIT Kanpur, September 24, 2016

CV Raman Medal (2016) Lecture on ***Atoms and Molecules in a Confined Environment***, Annual General Meeting of the Indian National Science Academy, NISER, Bhubaneswar, December 29, 2016

Atoms and molecules in a confined environment, HansRaj Mahila Maha Vidyalaya, Jalandhar, January 16, 2017

Non-adiabatic interactions and geometric phase, Guru Nanak Dev University, Amritsar, January 27, 2017

Non-adiabatic interactions and geometric phase, Recent Advances in Multi-Electron Theory, Goa, February 9-12, 2017

Atoms and Molecules in a Confined Environment, 5<sup>th</sup> Modeling of Chemical and Biological (Re)activity, CLRI, Chennai, Feb. 18-21, 2017

Institution Building: the Story of IISERs, IISER Mohali, February 25, 2017

Symmetry and Pattern Formation in Flowers, Science Day, IIT Roorkee, February 28, 2017

Atoms and Molecules in a Confined Environment, Foundation Day Lecture, INST, Mohali, March 2, 2017

Symmetry and Pattern Formation in Flowers, DST-Max-Planck-Partner group meeting, IISER Mohali, March 4, 2017

Curiosity Driven Science: from our garden back to the Gondwana land, K S Krishnan Lecture, GS Hindu High School, Srivilliputtur, July 4, 2017

Chintan Shivir, Current Status of Higher Education in India, IISER Bhopal, November 3, 2017

Symmetry and Pattern Formation in Flowers, Vijyoshi 2017, IISER Kolkata December 11, 2017

Atoms and molecules in a confined environment, 22<sup>nd</sup> CRSI National Symposium, Pt. Ravishankar Shukla University, Raipur Feb. 1-4, 2018

Atoms and Molecules in a confined environment, SDMC2018, Dooars, February 15-18, 2018

Atoms and Molecules in a confined environment, International Conference on Systems and Processes in Physics, Chemistry and Biology, Assam University, Silchar, March 1-3, 2018

Symmetry and Pattern Formation in Flowers – a multi-disciplinary approach, INSPIRE Programme, Panjab University, Chandigarh, March 28, 2018

Atoms and Molecules in a Confined Environment, Colloquium at IISER Tirupati, August 17, 2018

Academy lecture workshop on quantum chemistry and spectroscopy, SGGS Khalsa college, Mahilpur, September 28-29, 2018

Stabilising influence of silicon on benzene dimer and its isomers, International conference on frontiers at the chemistry – allied sciences interface, University of Rajasthan, Jaipur, December 21-22, 2018

The chemical bond, Modern trends in chemical sciences including green chemistry, SRM University, Chennai, December 27, 2018

Blue shifts due to confinement, Madurai Kamaraj University, Madurai, January 4, 2019

## **Abroad**

INDO-Japan workshop on spectroscopy and dynamics, Kobe, Japan September 25-27, 2006

Stacking and spreading interaction in N-heteroaromatic systems, Invited Lecture in the 2<sup>nd</sup> Indo-German Symposium on "Modeling Chemical and Biological (Re)activity, Wildbad Kreuth, Germany, October 4-7, 2009

Playing with the buckyball, XVIII European Conference on Dynamics of Molecular Systems, Curia/Andia, Portugal, September 5-10, 2010

(i) Indian Initiatives in Science Education, (ii) Chemistry: melting boundaries, Nepal Academy of Science and Technology, Kathmandu, April 7-8, 2011

Indian Initiatives in Science Education, Bangladesh Academy of Sciences, Dhaka, Bangladesh, May 9, 2011

Playing with the buckyball, Quaid Azam University, Islamabad, Pakistan, January 2012

Non-adiabatic interaction and the geometric phase, Jerusalem Nonadiabatica 2018, Hebrew University, Jerusalem, Israel, March 12-15, 2018

## **Seminars: India**

School of Chemistry, University of Hyderabad March 10, 1982

National Chemical Laboratory, Pune December 7-8, 1983

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore December 1-3, 1984

N.V.Subbarao Memorial Lecture, Department of Chemistry, Osmania University, Hyderabad March 22, 1988

School of Chemistry, Madurai Kamaraj University Sep. 30, 1989

National Chemical Laboratory, Pune Jan. 23, 1991

Department of Chemistry, Gorakhpur University, Jan. 18, 1992

Department of Chemistry, Univ. Roorkee, March 13, 1992

Regional Research Laboratory, Trivandrum, March 16-17, 1992

Department of Chemistry, Univ. Jammu March 30, 1992

Department of Chemistry, Banaras Hindu University, Varanasi, April 4, 1992

Central Leather Research Institute, Madras May 1995

Regional Research Laboratory, Trivandrum Dec. 4, 1996

Department of Chemistry, Panjab University, Chandigarh, August 2, 1999

R. P. Mitra Memorial Lecture, Department of Chemistry, Delhi University, Delhi Feb. 14, 2002

Department of Chemistry, Guru Nanak Dev University, Amritsar, 2003

Department of Chemistry, Gorakhpur University, Gorakhpur, Nov. 23-24, 2002

Department of Physics, Banaras Hindu University, Varanasi, 2004

Department of Chemistry Banaras Hindu University, Varanasi, August 2004

Department of Physics, Kumaun University, Nainital December 5, 2005

School of Chemistry, University of Hyderabad, Hyderabad March 14, 2006

Tata Institute of Fundamental Research, Mumbai October 11, 2006

Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati, May 2007

Physical Research Laboratory, Ahmedabad December 12, 2007

INSA local chapter, Department of Chemistry, Panjab University, Chandigarh January 24, 2008

Department of Chemistry, National Institute of Technology, Jalandhar, Sept. 29, 2008

Structural motifs in chemistry and chemical biology, NISER, Bhubaneswar, Feb. 20, 2014

### **Seminars: Abroad**

Hahn-Meitner Institut, Berlin August 30, 1982

Max-Planck-Institut fuer Stroemungsforschung, Goettingen FRG September 6, 1982

Department of Chemistry, University of Toronto, Toronto Canada February 1983

Chemistry Division, National Research Council, Ottawa, Canada April 22, 1983

Department of Chemistry, Oklahoma State University, Stillwater OK USA June 22, 1984

Institut fuer Physikalische Chemie der Universitaet Wuerzburg, FRG June 30, 1986

Fakultaet fuer Physik, Universitaet Bielfeld, FRG October 17, 1986

Fakultaet fuer Physik, Universitaet Kaiserslautern, FRG October 30, 1986

Max-Planck-Institut fuer Stroemungsforschung, Goettingen FRG November 5, 1986

Hahn-Meitner-Institut, Berlin April 27, 1987

H.C. Oersted Institut, Univ. Copenhagen, Denmark May 18, 1987

Department of Chemistry, Penn. State University, USA October 10, 1988

Surface Science Division, National Institute of Standards and Technology, Gaithersburg, USA October 12, 1988

Institut fuer Festkoerperphysik, Kernforschungsanlage, Juelich, FRG May 19, 1989

Facultaet fuer Physik, Albert-Ludwigs-Universitaet, Freiburg, FRG May 31, 1989

Department of Chemistry, State Univ. of New York, StonyBrook, New York, USA, July 3, 1989

Department of Chemistry, Stanford University, Stanford, Ca, USA, July 14, 1989

Surface Science Division, National Inst. Standards and Technology, Gaithersburg, Md, USA June 6, 1990

Dipartimento di Chimica, Universita di Roma, Italy June 19, 1990

Dipartimento di Chimica, Universita di Perugia, Italy June 22, 1990

National Institute of Standards and Technology, Gaithersburg, Md, USA July 7, 1994

Institut fuer Physikalische und Theoretische Chemie, Freie Universitaet Berlin, Berlin, Germany, April 23, 1996

Fachbereich Chemie, Universitaet Potsdam, Potsdam, Germany, April 23, 1996

Graduate School of Human Informatics, Nagoya University, Nagoya, Japan October 24, 1996

Institute of Molecular Science, Okazaki, Japan, Oct. 30, 1996



Department of Chemistry, Tohoku University, Sendai, Japan, Nov. 1, 1996

Faculty of Engineering, Tokyo University, Hongo, Japan, Nov. 6, 1996

National Institute of Standards and Technology, Gaithersburg Md, USA June 11, 1997

Department of Chemistry, Northwestern University, Evanston, IL, USA June 18, 1997

Departimento di Chimica, Universita di Roma, Italy, May, 2000

Dipartimento di Chimica, Universita di Perugia, Italy, May 2000

Department of Chemistry, University College, London, UK Nov. 30 – Dec. 1, 2000

Department of Chemistry, University of Oxford, Oxford, UK Dec. 4, 2000

Department of Chemistry, University of Cambridge, Cambridge, UK Dec. 6, 2000

Department of Chemistry, University of Bristol, Bristol, UK Dec. 8, 2000

Department of Chemistry, University of Manchester, Manchester, UK Dec. 12, 2000

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School of Environmental Sciences, Saitama University, Saitama, Japan August 8, 2017

Structural Motifs in Chemistry and Chemical Biology, Institute of Organic chemistry and Biochemistry, Prague, October 25, 2017

## Publications of Dr. N. Sathyamurthy

1. Quasiclassical trajectory studies using 3D spline interpolation of ab initio surfaces, N. Sathyamurthy and L. M. Raff, J. Chem. Phys. **63**, 464-473(1975).
2. Comparison of quantum mechanical and quasiclassical scattering as a function of surface topology, G. E. Kellerhals, N. Sathyamurthy and L. M. Raff, J. Chem. Phys. **64**, 818-825(1976).
3. Quantum mechanical scattering studies using 2D spline interpolation of a potential-energy surface, N. Sathyamurthy, G. E. Kellerhals and L. M. Raff, J. Chem. Phys. **64**, 2259-2261(1976).
4. Reactive scattering calculations on a spline-fitted ab initio surface:  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$  reaction, N. Sathyamurthy, R. Rangarajan and L. M. Raff, J. Chem. Phys. **64**, 4606-4611(1976).
5. Inelastic scattering calculations in polyatomic systems using an ab initio intermolecular potential-energy surface: The  $\text{CO}_2(0,0,1,0) + \text{H}_2(\text{D}_2) \rightarrow \text{CO}_2(0,0,0,0) + \text{H}_2(\text{D}_2)$  system, N. Sathyamurthy and L. M. Raff, J. Chem. Phys. **66**, 2191-2211(1977).
6. Quantum mechanical scattering calculations on a spline-fitted ab initio surface: The  $\text{He} + \text{H}_2^+ (v = 0, 1, 2) \rightarrow \text{HeH}^+ + \text{H}$  reaction, C. Stroud, N. Sathyamurthy, R. Rangarajan and L.M. Raff, Chem. Phys. Letters **48**, 350-353(1977).
7. On the origin of the dynamical differences on the diatomics-in-molecules and spline-fitted ab initio surfaces for the  $\text{He} + \text{H}_2^+$  reaction, N. Sathyamurthy, J. W. Duff, C. Stroud and L.M. Raff, J. Chem. Phys. **67**, 3563-3569(1977).
8. Rotational energy transfer (Theory) I. Comparison of quasiclassical and quantum mechanical results for elastic and rotationally inelastic HCl-Ar collisions, J. C. Polanyi, N. Sathyamurthy and J. L. Schreiber, Chem. Phys. **24**, 105-110(1977).
9. Rotational energy transfer (Theory) II. HCl + He, Ar, J. C. Polanyi and N. Sathyamurthy, Chem. Phys. **29**, 9-29 (1978).
10. Location of energy barriers VII. Sudden and gradual late-energy barriers, J. C. Polanyi and N. Sathyamurthy, Chem. Phys. **33**, 287-304(1978).
11. Effect of potential-well in an endothermic system: Reactive and vibrationally inelastic  $\text{He} + \text{H}_2^+$  collisions, N. Sathyamurthy, Chem. Phys. Letters **59**, 95-99(1978).
12. Rotational energy transfer (Theory) III. HCl + HCl, J. C. Polanyi and N. Sathyamurthy, J. Phys. Chem. **83**, 978-983(1979).

13. Location of energy barriers VIII. Reagent  $\rightarrow$  Product energy conversion on surfaces with sudden or gradual late-barriers,  
J. C. Polanyi and N. Sathyamurthy, Chem. Phys. **37**, 259-264(1979).
14. Reaction rate, rate constant and activation energy,  
N. Sathyamurthy, Indian J. Chem. Edn. **6**(2), 1-4(1979).
15. Inelastic scattering calculations in polyatomic systems using an ab initio intermolecular potential-energy surface II. Rotational energy transfer in CO<sub>2</sub>-H<sub>2</sub> collisions,  
N. Sathyamurthy and L. M. Raff, J. Chem. Phys. **72**, 3163-3178(1980).
16. Exponential gap relation and the rotational inelasticity of H<sub>2</sub>-M systems,  
C. Gayatri and N. Sathyamurthy, Chem. Phys. **48**, 227-235(1980).
17. Molecular collisions and chemical reactions,  
N. Sathyamurthy, Sci. Acad. Medal for Young Scientists - Lectures 1980, 17-20.
18. Negative activation energy for the Cl(Br)O + NO  $\rightarrow$  Cl(Br)O + NO<sub>2</sub> reactions,  
A. Menon and N. Sathyamurthy, J. Phys. Chem. **85**, 1021-1023(1981).
19. On the validity of the power gap law for rotational energy transfer in CO<sub>2</sub>-H<sub>2</sub> collisions,  
I. NoorBatcha and N. Sathyamurthy, Chem. Phys. Letters **79**, 264-268(1981).
20. Importance of correlation energy in collision dynamics: Quasiclassical trajectory study of collinear He + H<sub>2</sub><sup>+</sup> (v')  $\rightarrow$  HeH<sup>+</sup> + H using HF and CI potential-energy surfaces, N. Sathyamurthy, Chem. Phys. **62**, 1-19(1981).
21. Computer studies of molecular collisions and chemical reactions: A state-of-the-art survey,  
N. Sathyamurthy, Curr. Sci. **50**, 743-746(1981).
22. Effect of reagent rotation on cross section for the reaction Li + FH  $\rightarrow$  LiF + H,  
I. Noor-Batcha and N. Sathyamurthy, J. Am. Chem. Soc. **104**, 1766-1767(1982).
23. Vibrational threshold equal to the barrier height for an endothermic reaction: Li + FH  $\rightarrow$  LiF + H on an ab initio potential-energy surface,  
I. NoorBatcha and N. Sathyamurthy, J. Chem. Phys. **76**, 6447-6449(1982).
24. The challenge of fitting ab initio surfaces I. Rigid rotor CO<sub>2</sub>-H<sub>2</sub> potential,  
C. P. Shukla, A. K. Bachhawat and N. Sathyamurthy, Chem. Phys. **70**, 83-91(1982).
25. The challenge of fitting ab initio surfaces. A test of the utility of Akima's bivariate interpolation method to dynamical studies,  
S. K. Upadhyay and N. Sathyamurthy, Chem. Phys. Letters **92**, 631-636(1982).

26. Effect of the initial orientation of the reaction attributes for  $\text{Li} + \text{FH} \rightarrow \text{LiF} + \text{H}$  on an ab initio surface,  
I. NoorBatcha and N. Sathyamurthy, Chem. Phys. Letters **93**, 432-435(1982).
27. Dynamics of a prototype alkali-hydrogen-halide exchange reaction on an ab initio potential energy surface,  
I. NoorBatcha and N. Sathyamurthy, Chem. Phys. **77**, 67-91(1983).
28. Effect of reagent rotation on elementary bimolecular exchange reactions,  
N. Sathyamurthy, Chem. Rev. **83**, 601-618(1983).
29. On the origin of the dynamical differences between the Tang and Dalgarno-Henry-Roberts potentials for rigid rotor  $\text{H}_2$ -H collisions,  
S. Margolies, B. A. Garetz and N. Sathyamurthy, J. Chem. Phys. **79**, 2736-2741(1983).
30. Spectroscopy of the transition state (Theory) 3. Absorption by  $\text{H}_3^\ddagger$  in the three dimensional reaction  $\text{H} + \text{H}_2$ ,  
H. R. Mayne, J. C. Polanyi, N. Sathyamurthy and S. Raynor, J. Phys. Chem. **88**, 4064-4068(1984).
31. Three dimensional quasiclassical trajectory study of the reaction  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$  on an accurate ab initio potential-energy surface,  
T. Joseph and N. Sathyamurthy, J. Chem. Phys. **80**, 5332-5333(1984).
32. State-to-state chemistry: an ab initio approach,  
N. Sathyamurthy, Proc. Indian Acad. Sci. (Chem. Sci.) **93**, 449-457(1984).
33. Potential energy surface and molecular reaction dynamics,  
N. Sathyamurthy and T. Joseph, J. Chem. Educ. **61**, 968-971(1984).
34. Fitting repulsive potential-energy curves and surfaces,  
S. Thareja and N. Sathyamurthy, J. Chem. Soc., Faraday Trans.2, **81**, 717-723(1985).
35. Time-dependent wave mechanical study of the wings to the Lyman- $\alpha$  line in  $\text{H} + \text{H}_2$  reactive collisions,  
P. M. Agrawal, V. Mohan and N. Sathyamurthy, Chem. Phys. Letters **114**, 343-347(1985).
36. Rotational energy transfer in HF-Li collisions,  
K. Raghavan, S. K. Upadhyay, N. Sathyamurthy and R. Ramaswamy, J. Chem. Phys. **83**, 1573-1579(1985).
37. Computational fitting of ab initio potential-energy surfaces,  
N. Sathyamurthy, Computer Phys. Rep. **3**, 1-70(1985).
38. Quantum mechanical study of the collinear reaction  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ ,  
T. Joseph and N. Sathyamurthy, J. Indian Chem. Soc. **62**, 874-877(1985).

39. Time-dependent quantum mechanical approach to reactive scattering, V. Mohan and N. Sathyamurthy, *Current Sci.* **55**, 115-119(1986).
40. Absorption spectrum for the transition state  $H_3^\ddagger$  - A quantum mechanical model study, S. Sinha, N. Sathyamurthy and K. Banerjee, *Proc. Indian Acad. Sci.(Chem. Sci.)* **96**, 215-221(1986).
41. On the origin of the dynamical threshold for collision-induced dissociation processes, J. E. Dove, M. E. Mandy, N. Sathyamurthy and T. Joseph, *Chem. Phys. Letters* **127**, 1-6(1986).
42. Dynamics of the endothermic reaction  $He + H_2^+ \rightarrow HeH^+ + H$  on an accurate ab initio potential-energy surface, T. Joseph and N. Sathyamurthy, *J. Chem. Phys.* **86**, 704-714(1987).
43. Utility of the Sorbie-Murrell functional form in fitting the potential energy surface for the ground and the lowest excited state of  $H_3$ , S. Thareja and N. Sathyamurthy, *J. Phys. Chem.* **91**, 1790-1792(1987).
44. Nonlinear surprisal for product vibrational state distribution for the reaction  $Li + FH \rightarrow LiF + H$ , K. Raghavan, N. Sathyamurthy and R. D. Levine, *J. Mole. Struct. (Theochem)* **151**, 385-390(1987).
45. Dynamics of a model six-center exchange reaction, I. NoorBatcha, S. Thareja and N. Sathyamurthy, *J. Phys. Chem.* **91**, 2171-2173(1987).
46. Kinematic effects in rotationally inelastic  $A + BC$  collisions, K. Raghavan, N. Sathyamurthy and B. A. Garetz, *Chem. Phys.* **113**, 187-199(1987).
47. Resonances in collinear  $He + H_2^+$  collisions, N. Sathyamurthy, M. Baer and T. Joseph, *Chem. Phys.* **114**, 73-83(1987).
48. On the possibility of vibrational inhibition in a bimolecular exchange reaction, C. P. Shukla, N. Sathyamurthy and I. P. Khuller, *J. Chem. Phys.* **87**, 3251(1987).
49. Quantal wave packet calculations of reactive scattering, V. Mohan and N. Sathyamurthy, *Computer Phys. Rep.* **7**, 213-258(1988).
50. Investigation of the dependence of the  $Li_2$ -Na potential hypersurface on mean internuclear Li-Li distance, H.-G. Rubahn, N. Sathyamurthy and J. P. Toennies, *Faraday Disc. Chem. Soc.* **84**, 356-357(1988).
51. Effect of reagent rotation on the reaction  $D + H_2(v=1) \rightarrow DH + H$ , N. Sathyamurthy and J. P. Toennies, *Chem. Phys. Letters* **143**, 323-328(1988).

52. Collision-induced dissociation:  $\text{He} + \text{H}_2^+ \rightarrow \text{He} + \text{H} + \text{H}^+$ , S. Kumar and N. Sathyamurthy, *Indian J. Chem. Sci.* **2**, 1-5(1988).
53. Competition between exchange and dissociation processes in  $\text{He} + \text{H}_2^+$  collisions, S. Kumar and N. Sathyamurthy, *Chem. Phys.* **137**, 25-32 (1989).
54. Isotopic branching: experiment versus theory for  $\text{He} + \text{HD}^+$  collisions, K. C. Bhalla and N. Sathyamurthy, *Chem. Phys. Lett.* **160**, 437-442 (1989).
55. Time-dependent quantum mechanical study of  $\text{H}_2$  chemisorption on  $\text{W}(001)$ , S. Thareja and N. Sathyamurthy, *J. Indian Chem. Soc. special issue*, **66**, 596-598 (1989).
56. Fractals in molecule-surface collisions, V. Balasubramanian, N. Sathyamurthy and J. W. Gadzuk, *Surface Science Letters*, **221**, L741-749 (1989).
57. Maximization of entropy during a chemical reaction, N. Balakrishnan and N. Sathyamurthy, *Chem. Phys. Letters*, **164**, 267-269(1989).
58. Quasiclassical trajectory calculations of integral cross sections for highly vibrationally excited  $\text{Li}_2\text{-He}$ ,  $\text{Kr}$  systems, H.-G. Rubahn and N. Sathyamurthy, *Chem. Phys. Letters*, **171**, 506-512(1990).
59. Competition between dissociation and exchange processes: Contrasting dynamical behaviors in collinear  $\text{H}+\text{H}_2$  and  $\text{He}+\text{H}_2^+$  collisions, J. E. Dove, M. E. Mandy, V. Mohan and N. Sathyamurthy, *J. Chem. Phys.* **92**, 7373-81(1990).
60. Reactivity bands and fractals in model  $\text{H}_2\text{-W}(001)$  collisions, S. Thareja and N. Sathyamurthy, *Surface Science*, **237**, 266-272(1990).
61. Fractals in rotationally inelastic  $\text{HF-Li}$  collisions, S. Kumar and N. Sathyamurthy, *Chem. Phys. Letters*, **175**, 616-620(1990).
62. From alkali flames to automobile combustion: an illustration of the essential role of fundamental scientific research, N. Sathyamurthy, *Current Science*, **59**, 725-727(1990).
63. Time-dependent wave packet methods for the calculation of collinear atom-diatom exchange reaction probabilities, N. Balakrishnan and N. Sathyamurthy, *Computer Physics Communications*, **63**, 209-215(1991).
64. Probing the transition state, N. Sathyamurthy, in: *Reaction Dynamics: Recent Advances*, ed. N. Sathyamurthy, ch.2, Narosa, New Delhi and Springer-Verlag, Berlin (1991).
65.  $\text{HeH}_2^+$ : A case study in ab initio dynamics,

- N. Sathyamurthy, J. Indian Chem. Soc. **68**, 17-20(1991).
66. Fractals and resonances in collinear atom-diatom collisions,  
V. Balasubramanian and N. Sathyamurthy, Chemical Kinetics and Reaction Mechanism, ed. K.S. Gupta, RBSA Publishers, Jaipur (1991) p.73-79.
67. Fractals and resonances in collinear He + H<sub>2</sub><sup>+</sup> collisions,  
V. Balasubramanian, B.K. Mishra, A. Bahel, S. Kumar and N. Sathyamurthy, J. Chem. Phys. **95**, 4160-4167(1991).
68. Fractals in atomic and molecular collisions,  
N. Sathyamurthy, Current Science, **61**, 442- 446(1991).
69. Lasers in chemical reaction dynamics,  
N. Sathyamurthy, in: Lasers in chemical and biological sciences, ed. P. Chopra and H.M. Chawla, Wiley Eastern, New Delhi(1992) p.19-29.
70. Order in disorder: the case of irregular scattering,  
N. Sathyamurthy, Proc. 8th National workshop on atomic and molecular physics, Hyderabad Dec. 6-12, 1990 ed. A.P. Pathak, Narosa, New Delhi (1992).
71. Energy dependence of collision characteristics in molecule-surface collisions,  
V. Balasubramanian, A. Bahel, I. P. Dubey, N. Sathyamurthy and J.W. Gadzuk, J. Phys. Chem. **96**, 7870-7873(1992).
72. Chaos and fractals in the turning point search problem,  
R. Chatterjee and N. Sathyamurthy, J. Chem. Phys. **97**, 7006- 7007(1992).
73. State resolved scattering of molecules in pendular states: ICl + Ar,  
B. Friedrich, H.-G. Rubahn and N. Sathyamurthy, Phys. Rev. Letters **69**, 2487-2490(1992).
74. Resonances in collinear (He, H<sub>2</sub><sup>+</sup>) collisions: A time-dependent quantum mechanical study,  
N. Balakrishnan and N. Sathyamurthy, Chem. Phys. Letters **201**, 294-300(1993).
75. Quasiclassical trajectory study of Li<sub>2</sub> (v ≤ 25, j ≤ 100) - Na exchange reaction,  
H.-G. Rubahn and N. Sathyamurthy, Mol. Phys. **78**, 1047-1056(1993).
76. (He, H<sub>2</sub><sup>+</sup>) Dynamics revisited,  
S. Kumar, N. Sathyamurthy and K. C. Bhalla, J. Chem. Phys. **98**, 4680-4689(1993).
77. Channel control in a chemical reaction. Vibrational enhancement of I\*/I branching ratio in HI photodissociation,  
C. Kalyanaraman and N. Sathyamurthy, Chem. Phys. Letters, **209**, 52-56(1993).
78. Channel control in chemical reactions,  
C. Kalyanaraman and N. Sathyamurthy, Current Sci. **65**, 319-322(1993).

79. Three dimensional time-dependent quantum mechanical study of the reaction  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ ,  
N. Balakrishnan and N. Sathyamurthy, Proc. Indian Acad. Sci. (Chem. Sci.), **106**, 531-538(1994).
80. Collisional excitation of very high rotational levels of HF in small angle scattering with  $\text{He}^+$  at  $E_{\text{lab}} = 25\text{-}50$  eV,  
T. Ruhaltinger, N. Sathyamurthy, J.P. Toennies and R.G. Wang, J. Chem. Phys., **100**, 8877-8883(1994).
81.  $(\text{He}, \text{H}_2^+)$  Dynamics: A phase portrait analysis,  
A. Rahaman and N. Sathyamurthy, J. Phys. Chem. **98**, 12481-12485(1994).
82. Photodissociation and predissociation processes in OH: A time-dependent quantum mechanical study,  
C. Kalyanaraman and N. Sathyamurthy, Chem. Phys. **187**, 219-226(1994).
83. Possible reaction of atomic nitrogen with  $\text{SF}_x(x=1\text{-}5)$  and  $\text{CF}_x(x=1\text{-}3)$  fragments from  $\text{N}_2\text{-SF}_6$  and  $\text{N}_2\text{-CF}_4$  discharges,  
S.V.K. Kumar, N. Sathyamurthy, S. Manogaran and S.K. Mitra, Chem. Phys. Letters, **222**, 465-470(1994).
84. Kinematic effects in chemical reactions,  
I. NoorBatcha and N. Sathyamurthy, Malays. J. Sci. **15B**, 35-40(1994).
85. Kinetic model for reduction of iron oxide in molten slags by iron-carbon melt,  
A. Pal, B. Deo and N. Sathyamurthy, Steel Research, **65**, 414-420(1994).
86. Correlation function approach to transition state resonances in collinear  $(\text{He}, \text{H}_2^+)$  collisions,  
S. Mahapatra and N. Sathyamurthy, J. Chem. Phys. **102**, 6057-6066(1995).
87. Time-dependent wave packet study of the collinear reaction  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ ,  
N. Balakrishnan and N. Sathyamurthy, Chem. Phys. Letters, **240**, 119-124(1995).
88. Transition state resonances in collinear  $(\text{H}^-, \text{H}_2)$  collisions,  
S. Mahapatra, N. Sathyamurthy, S. Kumar and F. A. Gianturco, Chem. Phys. Letters, **241**, 223-228(1995).
89. Photo-induced desorption in NO/Pt: A time-dependent quantum mechanical study,  
N. Chakrabarti, V. Balasubramanian, N. Sathyamurthy and J. W. Gadzuk, Chem. Phys. Letters, **242**, 490-498(1995).
90. Overcoming the zero point dilemma in quasiclassical trajectories -  $(\text{He}, \text{H}_2^+)$  as a test case,  
S. Kumar, N. Sathyamurthy and R. Ramaswamy, J. Chem. Phys. **103**, 6021-6028(1995).



91. Anomalous vibrational excitation in the small angle scattering of  $\text{He}^+$  from HCl at  $E_{\text{lab}} = 20\text{-}60$  eV,  
T. Ruhaltinger, J. P. Toennies, R. G. Wang, S. Mahapatra, I. NoorBatcha and N. Sathyamurthy, J. Phys. Chem. **99**, 15544-15550(1995).
92. Resonance Raman intensity analysis of polyatomic molecules,  
N. Biswas, S. Umapathy, C. Kalyanaraman and N. Sathyamurthy, Proc. Indian Acad. Sci. (Chem. Sci.), **107**, 233-244(1995).
93. Resonances in collinear  $\text{H}^- + \text{H}_2 \rightarrow \text{H}_2 + \text{H}^-$  reaction: energy resolved reaction probabilities by the time-dependent wave packet approach,  
S. Mahapatra and N. Sathyamurthy, J. Phys. Chem. **100**, 2759-2761(1996).
94. Chemical systems,  
N. Sathyamurthy, in: Complex Systems, ed. J. K. Bhattacharyya and A. K. Mallik, Narosa, New Delhi (1996), ch.4.
95. Quantum chaos in collinear ( $\text{He}, \text{H}_2^+$ ) collisions,  
S. Mahapatra, R. Ramaswamy and N. Sathyamurthy, J. Chem. Phys. **104**, 3989(1996).
96. Collinear ( $\text{He}, \text{HD}^+$ ) and ( $\text{He}, \text{DH}^+$ ) collisions: transition state resonances and dynamics by time-dependent quantal wave packet approach,  
S. Mahapatra and N. Sathyamurthy, J. Chem. Phys. **105**, 10934(1996).
97. Possibility of proton oscillations through the benzene ring,  
R. S. Shresth, R. Manickavasagam, S. Mahapatra and N. Sathyamurthy, Current Sci. **71**, 49-50(1996).
98. Resonance deenhancement in the continuum Raman spectrum of HI,  
N. Chakrabarti, C. Kalyanaraman and N. Sathyamurthy, Chem. Phys. Letters, **267**, 31-36(1997).
99. Time-dependent quantum mechanical approach to reactive scattering and related processes,  
N. Balakrishnan, C. Kalyanaraman and N. Sathyamurthy, Physics Reports, **280**, 79-144(1997).
100. Negative imaginary potentials in time-dependent quantum molecular scattering,  
S. Mahapatra and N. Sathyamurthy, J. Chem. Soc. Faraday Trans. **93**, 773-779(1997).
101. Resonances and chaos in the collinear collision system ( $\text{He}, \text{H}_2^+$ ) and its isotopic variants,  
S. Mahapatra, N. Sathyamurthy and R. Ramaswamy, Pramana, **48**, 411(1997).
102. Autocorrelation function and its unifying role in structure and dynamics,  
S. Mahapatra, N. Chakrabarti, C. Kalyanaraman and N. Sathyamurthy, in: Atomic and Molecular Physics, ed. S.P. Khare, Deo Raj and A. Kumar, Bindra Publications, Ghaziabad, India, 1997, p.59-69.

103. Resonances in  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$  reaction in three dimensions: Energy resolved reaction probabilities by the time-dependent wave packet method,  
S. Mahapatra and N. Sathyamurthy, *J. Chem. Phys.* **107**, 6621(1997).
104. Photo-induced desorption of molecules from metal surfaces using femtosecond pulses: A model dynamical study,  
N. Chakrabarti, N. Sathyamurthy and J.W. Gadzuk, *J. Phys. Chem.A* **102**, 4154(1998).
105. Validation of photodissociation models using Raman excitation profiles: An application to IBr,  
Vandana, K., N. Chakrabarti, N. Sathyamurthy and M. K. Mishra, *Chem. Phys. Letters*, **288**, 545-552(1998).
106. Dynamics of the reaction  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$  on the Aguado-Paniagua surface,  
S. Kumar, H. Kapoor and N. Sathyamurthy, *Chem. Phys. Letters* **289**, 361-366(1998).
107. Classical mechanical investigations of collinear  $\text{H}^- + \text{H}_2 \rightarrow \text{H}_2 + \text{H}^-$  dynamics,  
W. H. Ansari and N. Sathyamurthy, *Chem. Phys. Letters* **289**, 487-493(1998).
108. An interesting isotope effect in the Raman excitation profile for HI,  
N. Chakrabarti and N. Sathyamurthy, *J. Phys. Chem. A*, **102**, 7089-7092(1998).
109. Exploring molecular motions in collinear  $\text{HeH}_2^+$  and its isotopic variants using periodic orbits,  
P. Bhatia, B. Maiti, N. Sathyamurthy, S. Stamatiadis and S. C. Farantos, *Phys. Chem. Chem. Phys.* **1**, 1105-1113(1999).
110. Ground and excited state intramolecular proton transfer in salicylic acid: An ab initio electronic structure investigation,  
S. Maheswari, A. Chowdhury, N. Sathyamurthy, H. B. Tripathi, M. Panda and J. Chandrasekhar, *J. Phys. Chem A* **103**, 6257-6268(1999).
111. Time correlation function and its unifying role in molecular structure and dynamics, S. Mahapatra, N. Chakrabarti and N. Sathyamurthy, *Int. Rev. Phys. Chem.* **18**, 235-262(1999).
112. Reduced potential energy curves for diatomic molecules and their respective cations, R. Abrol, N. Sathyamurthy and M. K. Harbola, *Chem. Phys. Letters* **312**, 341-345(1999).
113. Isotopic branching in  $(\text{He}, \text{HD}^+)$  collisions: a time-dependent quantum mechanical study in three dimensions,  
C. Kalyanaraman, D.C. Clary and N. Sathyamurthy, *J. Chem. Phys.* **111**, 10910-10918(1999).
114. Possibility of proton motion through buckminsterfullerene,  
S. Maheshwary, D. Chakraborty and N. Sathyamurthy, *Chem. Phys. Letters* **315**, 181-186(1999).
115. Dynamics of  $(\text{He}, \text{H}_2^+)$  collisions,  
B. Maiti and N. Sathyamurthy, *Proc. Indian Natl. Sci. Acad. A.* **66**, 59-70(2000).

116. Periodic orbit analysis for  $\text{HeH}_2^+$  in three dimensions,  
B. Maiti, N. Sathyamurthy, S. Stamatiadis and S. C. Farantos, *Indian J. Chem.* **39A**, 338-344(2000).
117. A time-dependent quantum mechanical investigation of dynamical resonances in three dimensional  $\text{HeH}_2^+$  and  $\text{HeHD}^+$  systems,  
B. Maiti, S. Mahapatra and N. Sathyamurthy, *J. Chem. Phys.* **113**, 59-66(2000).
118. Photochromism and photoreactivity of 2, 6-dichloro-4-methyl-3-pyridinecarboxaldehyde in the solid state,  
T. K. Sarkar, S. K. Ghosh, J. N. Moorthy, J.-M. Fang, S. K. Nandy, N. Sathyamurthy and D. Chakraborty, *Tetrahedron Letters* **41**, 6909-6913(2000).
119. Nonlinear phenomena in chemistry: channel control and mode selectivity in chemical reactions,  
N. Sathyamurthy, in: *Nonlinear Phenomena*, ed. S. K. Malik, M. K. Chandrashekar, N. Pradhan, Indian National Science Academy, New Delhi, 2000, pp. 931-946.
120. Photoinduced proton transfer in 3-hydroxy-2-naphthoic acid,  
H. Mishra, H.C. Joshi, H. B. Tripathi, S. Maheshwari, N. Sathyamurthy, M. Panda and J. Chandrasekhar, *J. Photochem. Photobiol.* **139**, 23-36(2001).
121. Bound and quasibound states of  $\text{HeH}_2^+$  and its isotopomers,  
B. Maiti and N. Sathyamurthy, *Chem. Phys. Letters* **345**, 461-470(2001).
122. Structure and stability of water clusters  $(\text{H}_2\text{O})_n$ ,  $n = 8-20$ : An ab initio investigation, S. Maheshwari, N. Patel, N. Sathyamurthy, A. D. Kulkarni and S. R. Gadre, *J. Phys. Chem. A* **105**, 10525 - 10537(2001).
123.  $\text{HeH}_2^+$ : A case study in time-dependent quantum mechanical approach to reactive scattering,  
B. Maiti and N. Sathyamurthy, in: "Time-dependent quantum dynamics", Ed. S. C. Althorpe, P. Soldán and G. G. Balint-Kurti, CCP6, 2001 p. 32-35.
124. Rotational isomers of 1-methoxynaphthalene: A combined study by ultraviolet laser spectroscopy in supersonic jet and ab initio theoretical calculation,  
K. K. Mahato, A. Das, A. N. Panda, T. Chakraborty and N. Sathyamurthy, *J. Phys. Chem. A* **106**, 12058-12063, 2002.
125. Reaction probabilities and reaction cross sections for three dimensional  $\text{He} + \text{H}_2^+$  ( $v$ ) collisions: A time-dependent quantum mechanical study,  
B. Maiti, C. Kalyanaraman, A. N. Panda and N. Sathyamurthy, *J. Chem. Phys.* **117**, 9719-9726, 2002.
126. Time-dependent density functional theoretical study of low lying excited states of  $\text{F}_2$ ,

- U. Lourderaj, M. K. Harbola and N. Sathyamurthy, Chem. Phys. Letters **366**, 88, 2002.
127. Solid state photochemistry of methyl-substituted pyridine-3-carboxaldehyde. Conformational control, structure-reactivity correlation and uv-vis spectroscopic characterization of photo-enols, Prasenjit Mal, U. Lourderaj, Parveen, P. Venugopalan, J. Narasimha Moorthy and N. Sathyamurthy, J. Org. Chem. **68**(2003)3446.
128. Reactive scattering resonances in (He, H<sub>2</sub><sup>+</sup>) collisions, B. Maiti and N. Sathyamurthy, in: Current Developments in Atomic, Molecular and Chemical Physics with Applications, Ed. Man Mohan, Kluwer, 2003.
129. Theory of atom-diatom scattering, N. Sathyamurthy, in Frontiers in Atomic, Molecular and Optical Physics, Vol. 3, Ed. S. C. Mukherjee and S. S. Bhattacharyya, Allied Publishers, New Delhi, 2003, p. 269-278.
130. Bound and quasibound states of He<sub>2</sub> H<sup>+</sup> and He<sub>2</sub>D<sup>+</sup> A. N. Panda and N. Sathyamurthy, J. Phys. Chem. A **107**, 7125-7131, 2003.
131. Possible explanation for the extended UV emission lines from helium-hydrogen plasma. N. Sathyamurthy, Current Science, **85**, 856, 2003.
132. Dynamics of (H<sup>-</sup>, H<sub>2</sub>) collisions: A Time-dependent quantum mechanical investigation on a new ab initio potential-energy surface, A. N. Panda and N. Sathyamurthy, J. Chem. Phys. **121**, 9343-9351(2004).
133. Chemical Reaction Dynamics: A time-dependent quantum mechanical approach A. N. Panda and N. Sathyamurthy, Proc. Indian Natn. Sci. Acad. **70A**, 635-648(2004).
134. Ab initio potential-energy surface for HeF<sub>2</sub> in its ground electronic state U. Lourderaj and N. Sathyamurthy, Chem. Phys. **308**, 277-284(2005).
135. Time-dependent quantum mechanical wave packet study of the He + H<sub>2</sub><sup>+</sup>(v,j) → HeH<sup>+</sup> + H reaction A. N. Panda and N. Sathyamurthy, J. Chem. Phys. **122**, 054304(2005).
136. π – π interaction in pyridine B. K. Mishra and N. Sathyamurthy, J. Phys. Chem. A **109**, 6-8(2005).
137. Hydrogen bonding in phenol, water and phenol-water clusters, R. Parthasarathi, V. Subramanian and N. Sathyamurthy, J. Phys. Chem. A **109**, 843-850(2005).
138. Three dimensional quantum dynamics of (H<sup>-</sup>, H<sub>2</sub>) and its isotopic variants A. N. Panda, K. Giri and N. Sathyamurthy, J. Phys. Chem. A **109**, 2057-2061(2005).
139. An experimental and theoretical investigation of the photophysics of 1-hydroxy-2-naphthoic acid,

- H. Mishra, S. Maheshwary, H. B. Tripathi and N. Sathyamurthy, *J. Phys. Chem. A* **109**, 2746-2754(2005).
140. Stability in polysilanes for light emitting diodes,  
A. Sharma, U. Lourderaj, Deepak, N. Sathyamurthy and M. Katiyar, *Compu. Mat. Sci.* **33**, 206-211(2005).
141. Determination of stability and degradation in polysilanes by an electronic mechanism  
A. Sharma, U. Lourderaj, Deepak and N. Sathyamurthy, *J. Phys. Chem. B* **109**, 15860(2005).
142. Water clusters in a confined nonpolar environment  
C. N. Ramachandran and N. Sathyamurthy, *Chem. Phys. Letters* **410**, 348-351(2005)
143. Bowls, balls and sheets of boric acid clusters: The role of pentagon and hexagon motifs  
M. Elango, R. Parthasarathi, V. Subramanian and N. Sathyamurthy, *J. Phys. Chem. A* **109**, 8587-8593(2005).
144. Preferential scattering of one isotopomer over another in (He,HD<sup>+</sup>) collisions  
A. K. Tiwari and N. Sathyamurthy, *Chem. Phys. Letters.* **414**, 509-513(2005).
145. Atomic and molecular clusters: designer materials for the nanoworld  
M. Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran and N. Sathyamurthy, *Proc. Indian Natn. Sci. Acad.* **70A**, xxx(2005).
146. Blue shift in X-H stretching frequency of molecules due to confinement  
O. Shameema, C. N. Ramachandran and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 2-4(2006).
147. Isotopic branching in (He, HD<sup>+</sup>) collisions  
A. K. Tewari, A. N. Panda and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 389-395(2006).
148. Ground and excited states of the monomer and dimer of certain carboxylic acids  
U.Lourderaj and N. Sathyamurthy, *J.Phys. Chem. A* **110**, 2709-(2006).
149. Hydrogen bonding without borders: an atoms-in-molecules perspective  
R. Parthasarathi, V. Subramanian and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 3349-3351(2006).
150. Structure and stability of salicylic acid-water complexes and the effect of molecular hydration on the spectral properties of salicylic acid  
A. K. Tewari and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 5960-5964(2006).
151. Hydrogen peroxide clusters: The role of open book motif in cage and helical structures  
M. Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 6294-6300(2006).
152. Stacking interaction in pyrazine dimer  
B. K. Mishra and N. Sathyamurthy, *J. Theoretical and Computational Chemistry*, **5**, 609-619 (2006)

153. Beta-phenyl quenching of triplet-excited ketones: How critical is the geometry for deactivation?  
S. Samanta, B. K. Mishra, T. C. S. Pace, N. Sathyamurthy, C. Bohne and J. N. Moorthy, *J. Org. Chem.* **71**(2006)4453 - 4459.
154. Effect of reagent rotation on isotopic branching in (He, HD<sup>+</sup>) collisions  
A. K. Tiwari and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 11200-11207(2006).
155. Ab initio quantum chemical investigation of the ground and excited states of salicylic acid dimer  
Shruti Maheshwary, U. Lourderaj and N. Sathyamurthy, *J. Phys. Chem. A* **110**, 12662-12669(2006).
156. Rotational excitation in (H, H<sub>2</sub>) collisions: a quantum mechanical study  
K. Giri and N. Sathyamurthy, *J. Phys. B: At. Mol. Opt. Phys.* **39**(2006)4123-4130.
157. Influence of reagent rotation on (H, D<sub>2</sub>) and (D, H<sub>2</sub>) collisions: A quantum mechanical study  
K. Giri and N. Sathyamurthy, *J. Phys. Chem. A* **110**(2006)13843-13849.
158. Introducing a twist in carbon nanotubes  
C. N. Ramachandran and N. Sathyamurthy, *Current Science*, **91**(2006)1503-1505.
159. Solvation of H<sub>3</sub>O<sup>+</sup> by phenol: Hydrogen bonding vs.  $\pi$  complexation  
R. Parthasarathi, V. Subramanian, N. Sathyamurthy and J. Leszczynski, *J. Phys. Chem. A* **111**, 2-5(2007).
160. Van der Waals complexes of small molecules with benzenoid rings: Influence of multipole moments on their mutual orientation  
B.K. Mishra and N. Sathyamurthy, *J. Phys. Chem. A* **111**, 2139-2147(2007).
161. Time-Dependent Density Functional Theoretical Study of the Absorption Properties of BN – Substituted C<sub>60</sub> Fullerenes  
C. N. Ramachandran and N. Sathyamurthy, *J. Phys. Chem. A* **111**, 6901-6903(2007)
162. Quantum dynamics of (H, HD) collisions at low energies  
K. Giri and N. Sathyamurthy, *Chem. Phys. Letters*, **444**(2007)23-27.
163. Dissociative double ionization of CO<sub>2</sub>: Dynamics, energy levels and lifetime  
V. Sharma, B. Bapat, J. Mondal, M. Hochlaf, K. Giri and N. Sathyamurthy, *J. Phys. Chem. A* **111**, 10205-10211(2007).
164. Hydrogen bonding in protonated water clusters: An atoms in molecules perspective  
R. Parthasarathi, V. Subramanian and N. Sathyamurthy, *J. Phys. Chem. A* **111**, 13287-13290(2007).

165. Quantum chemical investigation of the reaction of O ( $^3P_2$ ) with certain hydrocarbon radicals  
A. Gupta, R. P. Singh, V. B. Singh, B. K. Mishra and N. Sathyamurthy, *J. Chem. Sci.* **119**, 457-465(2007).
166. Electron density topography, NMR and NBO analysis of water clusters  
R. Parthasarathi, V. Subramanian and N. Sathyamurthy,  
*Synthesis and Reactivity in Inorganic, Metal-Organic and Nano-Metal Chemistry, Special issue on water clusters*, **38**, 18-27 (2008).
167. Cation- $\pi$  interaction: To stack or to spread  
B. K. Mishra, V. K. Bajpai, V. Ramanathan, S. R. Gadre and N. Sathyamurthy, *Mol. Phys.* **106**(2008)1557-1566.
168. Structure, Energetics and Reactivity of Boric Acid Nanotubes: A Molecular Tailoring Approach  
M. Elango, V. Subramanian, A. P. Rahalkar, S. R. Gadre, N. Sathyamurthy, *J. Phys. Chem. A* **112**(2008)7699-7704.
169. Host-guest interaction in endohedral fullerenes  
C. N. Ramachandran, D. Roy and N. Sathyamurthy, *Chem. Phys. Lett.* **461**(2008)87-92.
170. The self-assembly of metaboric acid molecules into bowls, balls and sheets  
M. Elango, V. Subramanian and N. Sathyamurthy, *J. Phys. Chem. A* **112**(2008)8107-8115
171. Structure and Stability of Water Chains (H<sub>2</sub>O)<sub>n</sub>, n = 5-20  
R. Parthasarathi, M. Elango, V. Subramanian and N. Sathyamurthy, *J. Phys. Chem. A* **113**(2009)3744-3749
172. Structure and stability of spiro-cyclic water clusters  
M. Elango, V. Subramanian and N. Sathyamurthy, *J. Chem. Sci.* **121**(2009)839-848.
173. Guest species trapped inside carbon nanotubes  
C. N. Ramachandran, Dario De Fazio, N. Sathyamurthy, V. Aquilanti, *Chem. Phys. Letters* **473**(2009)146-150.
174. Importance of Coriolis coupling in isotopic branching in (He, HD<sup>+</sup>) collisions  
A. K. Tiwari, S. Kolakkandy and N. Sathyamurthy, *J. Phys. Chem. A* **113**(2009)9568-9574.
175. Synthesis of germanium encapsulated fullerene  
D. Roy, N. K. Tripathi, K. Ram and N. Sathyamurthy, *Solid State Commun.* **149**(2009)1244-1247.
176. Potential energy curves for neutral and multiply charged carbon monoxide  
P. Kumar and N. Sathyamurthy, *Pramana – J. Phys.* **74**(2010)49-55.
177. Stacking and spreading interaction in N-heteroaromatic systems  
B. K. Mishra, J. S. Arey and N. Sathyamurthy, *J. Phys. Chem. A* **114**(2010)9606-9616.

178. Germanium encaged fullerene-synthesis, extraction, theoretical calculation and their possible application  
D. Roy, B. Shastri, C. N. Ramachandran, B. K. Mishra, K. Mukhopadhyay, N. Sathyamurthy and K. U. Bhasker Rao, in: Germanium: Properties, Production and Applications, Editor: Regina V. Germano 2011 Nova Science Publishers, Inc. pp. 151-185.
179. Aromaticity and hydrogen storage capability of planar  $N_6^{4+}$  and  $N_4^{2-}$  rings: A conceptual DFT approach  
S. Duley, S. Giri, N. Sathyamurthy, R. Islas, G. Merino, P. K. Chattaraj, Chem. Phys. Letters **506** (2011) 315–320.
180. Theoretical studies of host-guest interaction in gas hydrates  
P. Kumar and N. Sathyamurthy, J Phys. Chem. A 2011, 115, 14276–14281  
[dx.doi.org/10.1021/jp2089565](https://doi.org/10.1021/jp2089565)
181. A Theoretical Investigation on the Effect of  $\pi$ - $\pi$  Stacking Interaction on  $^1H$  Isotropic Chemical Shielding in Certain Homo- and Heteronuclear Aromatic Systems  
M. Majumder and N. Sathyamurthy, Theo. Chem. Acc. (2012) 131:1092 DOI 10.1007/s00214-012-1092-3.
182. An accurate ab initio potential energy curve and vibrational bound states for the  $X^2\Sigma_u^+$  state of  $H_2^-$   
S. Srivastava, N. Sathyamurthy and A. J. C. Varandas, Chem. Phys. 398 (2012)160-167.
183. Collision-Induced Dissociation in (He,  $H_2^+$  ( $v = 0-2$ ;  $j = 0-3$ )) System: A Time-Dependent Quantum Mechanical Investigation  
S. Kolakkandy, K. Giri and N. Sathyamurthy, J. Chem. Phys. 136, 244312 (2012); doi: 10.1063/1.4729255
184. Photoabsorption of carbon monoxide: a time-dependent quantum mechanical study  
M. Majumder, N. Sathyamurthy, H. Lefebvre-Brion and G J Vazquez, J. Phys. B: At. Mol. Opt. Phys. **45** (2012)185101.
185. Radiative lifetimes of spin forbidden  $a^1\Delta \rightarrow X^3\Sigma^-$  and spin allowed  $A^3\Pi \rightarrow X^3\Sigma^-$  transitions and complete basis set extrapolated ab initio potential energy curves for the ground and excited states of  $CH^-$   
S. Srivastava and N. Sathyamurthy, J. Chem. Phys. 137, 214314 (2012).
186. CH- $\pi$  and  $\pi$ - $\pi$  interaction in benzene–acetylene clusters  
M. Majumder, B. K. Mishra, N. Sathyamurthy, Chem. Phys. Letters **557** (2013) 59–65
187. An ab initio quantum chemical investigation of the structure and stability of ozone-water complexes  
P. Kumar and N. Sathyamurthy, Chem. Phys. 415(2013)214-221.



188. Ab initio potential energy curves for the ground and low lying excited states and the effect of  $^2\Sigma^+$  states on  $\Lambda$ -doubling of the ground state  $X^2\Pi$  of  $\text{NH}^+$   
S. Srivastava and N. Sathyamurthy, *J. Phys. Chem. A* 117 (2013) 8623–8631. DOI: 10.1021/jp4027628
189. Density functional theoretic studies of host-guest interaction in gas hydrates  
P. Kumar, B. K. Mishra and N. Sathyamurthy, *Computational and Theoretical Chemistry* 1029 (2014)26-32.
190. Stabilization of  $\text{C}_{20}$  cage by encapsulation of  $\text{H}^+$  and  $\text{He}^{2+}$  ions  
R. P. S. Abhijit Kumar, S. Dev, B.K. Mishra and N. Sathyamurthy, *Curr. Sci.* 106(2014)1254-1258.
191. Ab initio potential energy curves for the ground and low lying excited states of OH and  $\text{OH}^-$  and a study of rotational fine structure in photodetachment  
S. Srivastava and N. Sathyamurthy, *J. Phys. Chem. A* 118(2014)6343; doi: 10.1021/jp409940m
192. Interpretation of the accidental predissociation of the  $E^1\Pi$  state of CO  
M. Majumder, N. Sathyamurthy, G. J. Vazquez, H. Lefebvre-Brion, *J. Chem. Phys.* 140(2014)164303; doi:10.1063/1.4871109
193. Encapsulation of paramagnetic diatomic molecules  $\text{B}_2$ ,  $\text{O}_2$  and  $\text{Ge}_2$  inside  $\text{C}_{60}$   
A. Equbal, S. Srinivasan, C.N. Ramachandran, and N. Sathyamurthy, *Chem. Phys. Letters*, 610–611 (2014) 251–255.
194. Living legends in Indian science. S. Ranganathan: an organic chemist and an artist by nature  
N. Sathyamurthy, *Curr. Sci.* 107(2014)1892-1896
195. Jahn-Teller and Coupled Jahn-Teller/Renner-Teller effects in the calculation of adiabatic-to-diabatic transformation angle for the lowest three  $^2A'$  states of  $\text{NH}_2$  (NHH)  
S. Srivastava, M. Baer and N. Sathyamurthy, *Mol. Phys.* 113(2015)436;  
<http://dx.doi.org/10.1080/00268976.2014.948089>
196. Interaction of rare gas dimers in the confines of a carbon nanotube  
P. Kumar, C. N. Ramachandran, B. K. Mishra, N. Sathyamurthy, *Chem. Phys. Letters*, 618 (2015) 42–45.
197. The influence of sugar-phosphate backbone on the stacking interaction in B-DNA helix formation  
S. Mittal, B. K. Mishra and N. Sathyamurthy, *Curr. Sci.* 108(2015)1126-1131.
198. Relative stabilities and the spectral signatures of stacked and hydrogen bonded dimers of serotonin  
S. Dev, K. Giri, M. Majumder and N. Sathyamurthy, *Mol. Phys.* 113(2015)2952; DOI: 10.1080/00268976.2015.1060365
199. A study of topological effects concerning the lowest  $A''$  and the three  $A'$  states for the  $\text{CO}_2^+$  ion

V. Dhindhwal, M. Baer, N. Sathyamurthy, J. Phys. Chem. A 120(2016)2999;

[dx.doi.org/10.1021/acs.jpca.5b08921](https://doi.org/10.1021/acs.jpca.5b08921)

200. IISERs: emerging science universities of India (guest editorial)

N. Sathyamurthy, Curr. Sci. 110, 747-748 (2016)

201. The effect of hydration on the cation –  $\pi$  interaction between benzene and various cations

V. Dhindhwal, N. Sathyamurthy, J. Chem. Sci. 128, 1597-1606 (2016).

202. How different is the borazine-acetylene dimer from the benzene-acetylene dimer? A matrix isolation infrared and ab initio quantum chemical study

Kanupriya Verma, K. S. Viswanathan, M. Majumder and N. Sathyamurthy, Mol. Phys. 115, 2637-2648 (2017) <http://dx.doi.org/10.1080/00268976.2017.1284357>

203. An obsession with numbers: quantifying quality, N. Sathyamurthy, Curr. Sci. 113, 7-8 (2017)

204. Nanoclusters of Cyanuric Acid, M. Elango, V. Subramanian and N. Sathyamurthy, J. Chem. Sci. (Special issue in honor of Charusita Chakravarty) 129, 873-881(2017)

205. Stabilisation of the [6]-prismane structure by silicon substitution, A. Equbal, S. Srinivasan and N. Sathyamurthy, J. Chem. Sci. (Special issue in honor of Charusita Chakravarty) 129, 911-917(2017)

206. Heat capacity of endohedral fullerenes,  $R_g@C_{60}$  ( $R_g = \text{He, Ne, Ar and Kr}$ ), A. Koner, C. Kumar and N. Sathyamurthy, Mol. Phys. (M. Baer Festschrift), 116, 2728-2735 (2018); doi: 10.1080/00268976.2018.1463468

207. Co-operativity in Non-Covalent Interactions in Ternary complexes: A Comprehensive Electronic Structure Theory Based Investigation, S. V. K. Panneer, M. K. Ravva, B. K. Mishra, V. Subramanian, N. Sathyamurthy, J. Mol. Model (2018) 24: 258. <https://doi.org/10.1007/s00894-018-3796-3>

208. Stabilising influence of silicon substitution on dibenzene and its isomers

A. Koner and N. Sathyamurthy, J. Chem. Sci. (2019) doi.org/10.1007/s12039-018-1576-3

209. Influence of Stacking on the ground and excited states of 2-aminopyridine

A. Gupta, B. K. Mishra and N. Sathyamurthy, Computational and Theoretical Chemistry, 1148(2019)60-66.

209. Atoms and Molecules in a Confined Environment, PINSA- to be submitted.

210. Effect of molecular hydration on structure, stability and spectral properties of formic acid, acetic acid and benzoic acid

K. Giri and N. Sathyamurthy - to be published.

210. Aromaticity in two and three dimensions

Pallavika Ramaswamy and N. Sathyamurthy - to be published.

211. A real time study of the opening (anthesis) and closing of Passion Flower (*Passiflora incarnata*)

S. Sathyamurthy, S. Goyal and N. Sathyamurthy – to be published