

Mainak Sadhukhan

Curriculum Vitae

Personal informations

Date of birth 20 November 1983

Nationality Indian

Present affiliation

Position Assistant Professor

Tenure January, 2019 - present

Address FB-424
Department of Chemistry
IIT Kanpur,
Kanpur 208016

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Email mainaks@iitk.ac.in

Previous affiliations

April, 2016 - Postdoctoral research associate
December, C/O: Prof. Alexandre Tkatchenko
2018 Physics and Material Science Research Unit
University of Luxembourg

January, Royal Society Newton International Fellow
2014 - C/O: Prof. Frederick Roy Manby
December, Centre for Computational Chemistry
2015 Department of Chemistry
University of Bristol

July, 2013 - Postdoctoral Research Associate -I
December, C/O: Prof. R. Biswas
2013 Department of Chemical, Biological and Macromolecular Sciences
S. N. Bose National Centre for Basic Sciences

May, 2013 - Visiting Scholar
July, 2013 C/O: Prof. P. K. Panigrahi
Department of Physical Sciences
Indian Institute of Science Education and Research-Kolkata

February, Visiting Scholar
2013 - May, C/O: Prof. A. K. Roy
2013 Department of Chemical Sciences
Indian Institute of Science Education and Research-Kolkata

February, Senior Research Fellow (CSIR)
2010 - C/O: Prof. B. M. Deb
January, Department of Chemical Sciences
2013 Indian Institute of Science Education and Research-Kolkata

February, Junior Research Fellow (CSIR)
2008 - C/O: Prof. B. M. Deb
January, Department of Chemical Sciences
2010 Indian Institute of Science Education and Research-Kolkata

November, Institute Research Fellow (CSIR-LS)
2007 - C/O: Prof. B. M. Deb
January, Department of Chemical Sciences
2008 Indian Institute of Science Education and Research-Kolkata

Grants and fellowships

2016-2017 Royal Society Newton International Fellowship Alumnus Research Grant

2014-2015 Royal Society Newton International Fellowship Research Grant

2008-2013 CSIR Research Fellowships

Academic qualifications

Doctor of Philosophy (PhD) Date : 1st July, 2013
Thesis : Atoms and molecules under strong external fields
Supervisor: Prof. B. M. Deb

Master of Science (M.Sc.) Year: 2007
Subject: Chemical Sciences
Institution: S. N. Bose National Centre for Basic Sciences
Affiliation: West Bengal University of Technology

Bachelor of Science (B.Sc.) Year: 2005
Major subject: Chemistry (Hons.)
Subsidiary subjects: Mathematics and Physics
Class I
Institution: Presidency College, Kolkata
Affiliation: University of Calcutta

Areas of expertise

Theoretical Chemistry, Chemical Physics, Soft condensed matter physics, Noncovalent interactions, Strong-field electron dynamics, Nonlinear dynamics, Quantum chaos, Quantum dynamics, Electron structure theory

Complete list of publications

- 2018 Mainak Sadhukhan and Alexandre Tkatchenko. Sadhukhan and tkatchenko reply. *Physical Review Letters* 120,258902 (2018).
- 2018 Mainak Sadhukhan and B. M. Deb. An investigation into possible quantum chaos in the H₂ molecule under intense laser fields via Ehrenfest phase space (EPS) trajectories. *Journal of molecular modelling* 24,169 (2018).
- 2018 D. V. Fedorov, Mainak Sadhukhan, Martin Stöhr, and Alexandre Tkatchenko. Quantum-mechanical relation between atomic dipole polarizability and the van der waals radius. *Physical Review Letters* (2018). (accepted).
- 2017 Mainak Sadhukhan and Alexandre Tkatchenko. Long-range repulsion between spatially confined van der waals dimers. *Physical Review Letters* 118,210402 (2017).

- 2017 M. Sadhukhan and B. M. Deb. Ehrenfest “phase-space” trajectories and quantum chaos in He atom under strong, oscillating magnetic fields : An application of time-dependent quantum fluid density functional theory (TDQFT). *Molecular Physics* 115,815 (2017).
- 2016 M. Sadhukhan, Amlan K Roy, P. K. Panigrahi, and B. M. Deb. Dynamics of electronic motion in hydrogen atom under parallel strong oscillating magnetic field and intense laser fields. *International Journal of Quantum Chemistry* 116,377 (2016).
- 2016 M. Sadhukhan and Frederick R. Manby. Quantum mechanics of drude oscillators with full coulomb interaction. *Physical Review B* 94,115106 (2016).
- 2016 M. Sadhukhan and B. M Deb. Dynamical deformations of the electron density in an H₂ molecule under strong, oscillating magnetic fields: an application of time-dependent quantum fluid density functional theory. *Molecular Physics* 114,3490 (2016).
- 2014 M. Sadhukhan and B. M. Deb. Electron dynamics of a He atom in strong, oscillating magnetic fields. *Physical Review A* 89,042516 (2014).
- 2012 M. Sadhukhan and B. M. Deb. Atoms and molecules in strong magnetic fields. In Amlan K. Roy, editor, *Theoretical and Computational Developments in Modern Density Functional Theory*. Nova Science Publishers, New York (2012).
- 2011 M. Sadhukhan and B. M. Deb. A dynamical signature of quantum chaos in hydrogen atom under strong, oscillating magnetic fields. *Europhysics Letters* 94,50008 (2011).
- 2010 Mainak Sadhukhan and B. M. Deb. Variations in electron density and bonding in the lowest $^1\Sigma_g$ state of H₂ molecule under strong magnetic fields by using a time-dependent density functional theory. *Journal of Molecular Structure: THEOCHEM* 943,65 (2010).
- 2010 M. Sadhukhan, P. K. Panigrahi, and B. M. Deb. Dynamics of a hydrogen atom under a strong, time-dependent magnetic field. *Europhysics Letters* 91,23001 (2010).

- 2008 B. M. Deb, Mainak Sadhukhan, Sudarson Sekhar Sinha, Sucheta Sengupta, and Ranjit Biswas. An integrated and open-ended experiment. *Resonance* 13,54 (2008).
- 2007 Mainak Sadhukhan and B. M. Deb. Aspects of electron dynamics in a helium atom under an intense laser field. *Indian Journal of Physics* 81,969 (2007).

Invited talks

- 2015 Host: Prof. Alexandre Tkatchenko
Theory Department of the Fritz-Haber Institute
Berlin, Germany
- 2016 Host: Prof. Leeor Kronik
Department of material science and interface
Weizmann Institute of Science
Israel
- 2017 Host: Prof. Kenneth D. Jordan
Department of Chemistry
University of Pittsburgh
USA
- 2017 Host: Prof. Robert DiStasio Jr.
Department of Chemistry and Chemical Biology
Cornell University
USA
- 2017 Host: Prof. Pavel Hobza
Department of Computational Chemistry
Institute of Organic Chemistry and Biochemistry
Czech Republic
- 2018 Host: Dr. Hemant K. Kashyap
Department of Chemistry
Indian Institute of Technology - Delhi
India

Conference presentations

| Conference | Place | Year | Mode |
|---|---|------|-----------------|
| Theoretical Chemistry Symposium | IISc, Bangalore, India | 2009 | Poster |
| Of Molecules and Materials | IISER-Kolkata, India | 2009 | Poster |
| Inter-IISER Chemistry meet-2009 | IISER-Kolkata, India | 2009 | N. A. |
| Department of Chemical Sciences In-house seminar | IISER-Kolkata, India | 2010 | Oral |
| Department of Chemical Sciences Department Day | IISER-Kolkata, India | 2012 | Oral |
| DAE-BRNS symposium on Atomic, Molecular and Optical Physics | IISER-Kolkata, India | 2012 | Oral |
| Theoretical Chemistry Symposium | IIT-Guwahati, India | 2012 | Poster |
| Current Trends in Theoretical Chemistry | Bhabha Atomic Research Centre, India | 2013 | Poster |
| Computational Molecular Science | University of Warwick, UK | 2015 | Poster |
| American Physical Society March meeting | New Orleans, USA | 2017 | Oral |
| Telluride Science Research Center workshop on intermolecular interactions : New challenges for ab initio theory | Arenas de Cabrales-Picos de Europa, Spain | 2017 | Oral and Poster |
| American Physical Society March meeting | Los Angeles, USA | 2018 | Oral |
| Advanced Molecular Simulations | IIT Delhi, India | 2019 | Invited speaker |

Teaching experience

Tutor (2019) CHM 102A
 2nd semester undergraduate
 Indian Institute of Technology-Kanpur

Teacher(2016) Computational Physics
Masters in Physics
University of Luxembourg

Teaching Quantum Mechanics I
Assistant 1st semester, Masters of Science, Physical Sciences
(2013) S. N. Bose National Centre for Basic Sciences

Teaching Bonding, Structure and Symmetry
Assistant 4th semester BS-MS, Chemistry
(2008-2012) Indian Institute of Science Education and Research Kolkata

Teaching Indian Heritage in Science, Literature and Arts
Assistant 2nd semester BS-MS
(2008-2012) Indian Institute of Science Education and Research Kolkata