Sangita Sen

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CURRENT POSITION

Assistant Professor,
Dept. of Chemical Sciences, IISER, Kolkata — June, 2020-Present
Field: Theoretical Quantum Chemistry

PREVIOUS POSITION

Post-Doctoral Marie-Curie Research Fellow — 2016-2020
Hylleraas Centre for Quantum Molecular Science, University of Oslo, NORWAY
Project: Spectra of Molecules in Strong Magnetic Fields, with Dr. Erik Tellgren

EDUCATION

- ***PhD in Chemistry***
  In Theoretical and Computational Chemistry — 2010 – 2015
  Under Prof. Debashis Mukherjee and Dr. Ankan Paul
  Indian Association for the Cultivation of Science (IACS)
  Jadavpur University, Kolkata, INDIA

  Thesis: *' Multi-reference coupled-cluster studies on the effect of dynamical and non-dynamical correlation on molecular energies and properties'*

- ***Master of Science – Chemical Sciences (Int PhD Programme)***
  Indian Association for the Cultivation of Science (IACS)
  Kolkata, INDIA — 2008 – 2010

  Thesis: *'A Fock space approach to valence universal multi-reference perturbation theory for calculation of energy differences vis ionization potential and electron affinity'*

- ***Bachelor of Science (Honours) – Chemistry***
  Jadavpur University, Kolkata — 2005-2008
- ***High School***
  G. D. Birla Centre for Education, Kolkata — 2003-2005
- ***School***
  Loreto House, Kolkata — 1993-2003

ACADEMIC AWARDS AND FELLOWSHIPS

- **Editor's Choice, JCP, 2018** (72 articles out of all published in 2018) 2019
- **Editor's Pick Article, JCP** 2018
- **Best Poster Award** at APCTCC, Mumbai 2017
- **Marie Curie Individual Fellowship** 2017
- **Best Poster Award** at ICQC, Beijing 2015
- **Best Poster Award** at TCS, Pune 2014
- **Shyama Prasad Mukherjee Fellowship** awarded to 3 persons in India in the Chemical Science category that year 2010
- Placed **2nd in MSc** from IACS, Kolkata 2010
- Qualified GATE 2010 achieving 57th rank 2010
- Qualified CSIR-NET achieving **16th rank** 2009
- Placed **2nd in BSc** from Jadavpur University, Kolkata 2008
- Qualified IIT JAM, 2008 achieving 91st rank 2008
- Qualified for admission to IISc Bangalore for Integrated PhD in Chemistry achieving **1st position** in merit list 2008
- Qualified for admission to IACS, Kolkata for Integrated PhD in Chemistry achieving **1st position** in merit list 2008
- Received **KVPY fellowship** (Reg.No. 1051225) 2006-2010
- Received the Mamraj Agarwal Rastriya Puraskar (**Governor's Award**), for outstanding performance in the ISC (Class XII) examination (**Topper**) 2005
- Received the Reynold's Scholarship, 2004 for Academic Excellence 2004
- Received the Dr. Radha Binode Paul Memorial Trophy for Highest Achievement in Hist., Civics & Geog. in ICSE 2003

RESEARCH INTERESTS

- Quantum Computing for Quantum Chemistry
- Reaction Dynamics
- Study of changes in the excitation spectrum of molecules placed in magnetic fields
- Study of molecular bonding in magnetic fields
- Coupled-Cluster theories
- Spin adaptation of coupled cluster theories
- Conserving and Breaking Spin Symmetries
- High level computation of molecular potential energy surfaces, spectroscopic energy differences and electric and magnetic properties
- Development and application of multi-reference coupled cluster theories for atomic and molecular systems
- Developing pilot codes for these newly formulated theories
- Techniques for code optimisation
- Machine learning in Quantum Chemistry

PUBLICATIONS

- *"Reappraisal of the normal ordered Jeziorski-Monkhorst ansatz in the UGA-OSCC theory for a study of IP, EA and EE"*
  D. Chakravarti, S. Sen and D. Mukherjee, Mol. Phys., **119**, 21, (2021)

- *"Benchmarking Density Functional Approximations for Diamagnetic and Paramagnetic Molecules in Nonuniform Magnetic Fields"*
  S. Sen and E. Tellgren, J. Chem. Theory Comput., **17**, 1480 (2021)

- *"Excited States of Molecules in Strong Magnetic Fields"*
  S. Sen, K.K. Lange and E.I. Tellgren, J. Chem. Theory Comput. **15**, 3974 (2019)

- *"A local tensor that unifies kinetic energy density and vorticity in density functional theory"*
  S. Sen and E.I. Tellgren, J. Chem. Phys. **149**, 144109 (2018): **Editor's Choice 2018** (72 articles out of all published in 2018), **Featured article**,
  also selected for publication as popular science article in SciLight (AIP)

- *"Non-perturbative calculation of orbital and spin effects in molecules subject to non-uniform magnetic fields"*
  S. Sen and E.I. Tellgren, *J. Chem. Phys.,* **148**, 184112 (2018) : **Editor's Pick**

- *"Inclusion of Orbital Relaxation and Correlation through the Unitary Group Adapted Open Shell Coupled Cluster Theory using Non-relativistic and Scalar Relativistic Hamiltonians to study the Core Ionization Potential of Molecules containing Light to Medium-heavy elements"*
  S. Sen, A. Shee and D. Mukherjee, *J. Chem. Phys.,* **148**, 054107 (2018)

- *"Aspects of Size Consistency of Orbitally Non-invariant Size-extensive Multi-reference Perturbation Theories: A Case Study Using the UGA-SSMRPT2 as a Proto-type"*
  A.Sen, S. Sen and D. Mukherjee, *J. Chem. Theory Comput*., **11**, 4129 (2015)

- *"Unitary Group Adapted State Specific Multireference Perturbation Theory: Formulation and Pilot Applications"*
  A. Sen, S. Sen, P. K. Samanta and D. Mukherjee, *J. Comp. Chem*., **36**, 670, (2015) : **Inside Cover**

- *"Aspects of Size-extensivity in Unitary Group Adapted Multi-Reference Coupled Cluster Theories: The Role of Cumulant Decomposition of Spin-free Reduced Density Matrices"*
  R. Maitra, D. Sinha, S. Sen and D. Mukherjee, *Theor. Chem. Acc*., **133**, 1522 (2014)

- *"A study of the ionisation and excitation energies of core electrons using a unitary group adapted state universal approach"*
  S. Sen, A. Shee and D. Mukherjee, *Mol. Phys,* **111**, 2625 (2013)

- *"Exploration of Various Aspects of UGA-SUMRCC: Size Extensivity, Possible Use of Sufficiency Conditions, and an Extension for Direct Determination of Energy Differences"*
  A.Shee, S. Sen and D. Mukherjee, *J. Chem. Theory Comput.,* **9**, 2573 (2013)

- *"Formulation and implementation of a unitary group adapted state universal multi-reference coupled cluster (UGA-SUMRCC) theory: Excited and ionized state energies"*
  S. Sen, A. Shee and D. Mukherjee, *J. Chem. Phys.*, **137**, 074104 (2012)

- *"Recent Advances in Spin-Free State-Specific and State-Universal Multi-Reference Coupled Cluster Formalisms: A Unitary Group Adapted Approach"*
  R. Maitra, D. Sinha, S. Sen, A. Shee and D. Mukherjee *in*
  "Theory and Application in Computational Chemistry. The First Decade of the Second Millennium", AIP Conf Proc. **1456**, 81 (2012)

EARLIER PROJECTS

- *'To assess the breakdown of orbital picture: A study on C_2'*
  Prof. Debashis Mukherjee, IACS, Kolkata — Jul-Dec, 2009
- *'Synthesis of Dienophiles and Dienes, and their Diels-Alder reactions'*
  Prof. S. Lahiri, IACS, Kolkata — Sep-Oct, 2008
- *'Quenching of fluorescence of 2-anthracene sulphonate by Co^{2+} in aqueous and micellar solution of TritonX-114'*
  Prof. S. C. Bhattacharya, Jadavpur University — Jun-Jul, 2008
- *'Synthesis of a series of dinuclear Ruthenium complexes with dinucleating ligands'*
  Prof. Samaresh Bhattacharya, Jadavpur University — Jul-Sep, 2007

CONFERENCES AND SCHOOLS ATTENDED

• QSCP, Jaipur, India (**Invited Speaker**)	2023
•SDSS, Kolkata, India	2023
•APATCC, Quy Nhon, Vietnam (**Invited Speaker**)	2023
•RAC, Shillong, India (**Invited Speaker**)	2022
•SDMC, Udupi, India (**Invited Speaker**)	2022
•FORCE, Agra, India (**Invited Speaker**)	2022
•MNIT, Jaipur, India (**Invited Seminar**)	2022
•ITCC, IISERK, India (**Invited Speaker**)	2022
•QIQT, IISERK, India (**Invited Speaker**)	2022
•TCMSD, IACS, Kolkata (**Chair**)	2022
•CRSI Conference, India	2021
•ICFAI, Tripura University (**Invited Speaker**)	2021
•Theoretical Chemistry Symposium, Kolkata, India (**Invited Speaker**)	2021
•FSQT 2020 (Poster)	2020
•Hylleraas Friday Seminar	2020
•Geilo Winter School	2019
•MAGIC 2018, Serbia (**Invited Speaker**)	2018
•EMN Meeting on Computation and Theory, Spain (**Invited Speaker**)	2018
• Young CAS Workshop, Norway	2018
•CAS Final Meeting, Oslo, Norway (Poster)	2018
•CAS Mid-term Meeting, Oslo, Norway (Poster)	2018
•APCTCC, Mumbai, India (**Best Poster**)	2017
•WATOC, Munich, Italy (Poster)	2017
•Molecular Properties and Computational Spectroscopy, Pisa, Italy (**Speaker**)	2017
•Swedish Theoretical Chemistry, Lund, Sweden	2016
•CTCC Annual Meeting, Alta, Norway (**Speaker**)	2016
•International Congress of Quantum Chemistry, Beijing, China (**Best Poster**)	2015
•Recent Advances in Electronic Structure Theory, Nanjing, China (Poster)	2015
•Theoretical Chemistry Symposium, Pune, India (**Best Poster**)	2014
•Quantum Systems in Chemistry, Physics and Biology, Taipei, Taiwan (Poster)	2014
•Recent Advances in Correlation Problems, IACS, Kolkata	2013
•Electronic Structure and Dynamics of Molecules and Clusters, Kolkata (Poster)	2013
•International Congress of Quantum Chemistry, Boulder, USA (Posters)	2012
•Coupled-cluster Theory and Related Techniques, Boulder, Colorado, USA	2012
•Recent Advances in Many Electron Theories II, Puri (Poster)	2011
•School on Understanding Molecular Simulations, IIT Kanpur	2010
•Recent Advances in Many Electron Theories I, Shankarpur	2009
•KVPY Summer Programme, IISc, Bangalore with Prof. Anjali Kharande	2006

TECHNICAL SKILLS

- Linear Algebra, Matrix Operations, Numerical Methods
- Electronic Structure Theories: **Coupled-Cluster, Correlated Theories for Open-Shell systems** and **Excited States,** DFT, MCSCF, Multi-reference Perturbation Theories, Response Theories for **Molecular Properties**
- Computer languages: **FORTRAN 77, FORTRAN 90, C, C++**
- Development of a **package of programs (>80,000 lines)** from scratch for high level electron correlation theories, eg. Multi-Reference Coupled Cluster theories which can be used in conjunction with standard packages like GAMESS, DIRAC and LONDON
- Optimization of tensor operations
- Quantum Chemistry Package Programs: GAMESS, DALTON, DIRAC, LONDON, GAUSSIAN
- **Python scripting**, UNIX shell programming, LaTeX
- Basic skills in **Matlab, Gnuplot, Intel VTune Amplifier, GDB, Valgrind, Java**
- Basic knowledge of molecular simulations

TEACHING & SUPERVISION

- Current PhD students: 4, Masters Project: 2
- Courses taught at IISER Kolkata: Quantum Mechanics I, Advanced Quantum Chemistry, Principles of Spectroscopy, Chemical Kinetics, Research Methodology
- Co-supervision of Master's project at IACS, Kolkata (2015)
- Classroom instruction in Physics for classes 9 and 10 in St. Sebastian School, Kolkata (2007)

ADMINISTRATIVE RESPONSIBILITIES

- Cultural Secretary, CULTVISION (Scienfest)
- Student representative to the Governing Council, IACS, Kolkata
- Member of a PhD recruitment committee, Dept. of Chemistry, UiO

COLLABORATIVE PROJECTS

- Prof. Trygve Helgaker and Dr. Erik Tellgren CTCC, Oslo, Norway

  'Computation of magnetic properties of open shell molecules using spin-adapted coupled cluster theory' (2013-2019)

- Dr. Simen Reine, CTCC, Oslo, Norway

  'Development of automatic expression generator (AEG) and self-optimizing tensor contraction engine(TCE) for non-linear tensor multiplications in computationally intensive codes' (2013-2015)

- Prof. Trond Saue and Avijit Shee, Universite Paul Sabatier, Toulouse, France

  'Correlated studies of core electron ionization and excitation in the relativistic framework' (2013-2015)

- Prof. T. Daniel Crawford

  'Code development for analytic gradient of single reference coupled cluster theory' (2012)

REFERENCES

1. **Prof. Debashis Mukherjee**
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   Indian Association for the Cultivation of Science
   Raja S. C. Mullick Road, Jadavpur, KOLKATA 700 032, India
   Phone: +91 9331019518, +91 33 2473 4971 (Ext 1451)
   Email: pcdm@iacs.res.in , pcdemu@gmail.com

2. **Dr. Erik Tellgren**
   Researcher, Hylleraas Centre for Quantum Molecular Sciences
   Department of Chemistry Mobile ph. : +47 97406408
   University of Oslo
   P.O.Box 1033 Blindern
   N-0315 Oslo, Norway
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3. **Prof. Trygve Helgaker**
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4. **Prof. Trond Saue**
   Laboratoire de Chimie et Physique Quantiques
   UMR 5626 CNRS --- Université Toulouse III-Paul Sabatier
   118 route de Narbonne, 31062 Toulouse (FRANCE)
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PERSONAL DETAILS

Father's Name: Subir Ranjan Sen

Mother's Name: Sushmita Sen

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Marital Status: Married

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KOLKATA 700 029, India

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