Sudip Kumar Chattopadhyay

Contacts

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Department of Chemistry
Indian Institute of Engineering Science& Technology (IIEST) Shibpur
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Curriculum Vitae

Education

Ph. D. (Chemical Physics)	IACS, Kolkata, India (Jadavpur University)
M. Sc. (Physical Chemistry)	University of Burdwan, India
B. Sc. (Chemistry)	University of Burdwan, India

Awards/Honors /Recognition

1. Received the ***Dr.MrigendranathGhosh Medal*** from the University of Burdwan for securing **First Class First Position** **in *B. Sc. Hons*** *(Chemistry) Examination.*

2. Received the ***University Gold Medal***from the University of Burdwan for securing **First Class First Position** **in *M. Sc.****(Chemistry) Examination*.

3. Received the ***BardhamanSammilani Medal*** from the University of Burdwan for securing **First Class First Position** **in *M. Sc.*** *(Chemistry) Examination.*

4. **National Merit Scholarship** **(B. Sc)** awarded by the Department of Education, Ministry of Human Resource Development, Government of India

5. **Recipient of Young Faculty Research Award**-*2014***.**

Ph. D. Thesis

Title: ***Development and Application of State-specific Multireference Theories to Treat Response Properties of Strongly Correlated Molecular Systems.***

Advisor: **Professor Debashis Mukherjee**
Indian Association for the Cultivation of Science (IACS), Kolkata 700032, India

News-Highlights

1. **Book**: ***Many-body Methods for Atoms and Molecules by R. K. Chaudhuri and S. Chattopadhyay (CRC-Press: Taylor & Francis Group, 2016***).

2. Our paper "***Realization of a Brownian engine to study transport phenomena: A semiclassical approach***" [**Physical Review E (*American Physical Society*) 81**, 061112 (2010), doi:10.1103/PhysRevE.81.061112] has been cited as a "***RESEARCH HIGHLIGHT" in NATURE INDIA*** [doi:10.1038/nindia.2010.87; Published online 30 June 2010].

3. Chattopadhyay and co-workers have published an invited paper as part of The ***Molecular Physics*** -2020 "***Special Issue in Honour of JÜRGEN GAUSS***".

4. Chattopadhyay and co-workers have published an invited paper as part of The ***Molecular Physics*** -2017 "***Special Issue in Honour of Debashis Mukherjee***".

5. Chattopadhyay and co-workers have published an invited paper as part of The ***Journal of Physical Chemistry*** (**ACS**) virtual special issue "***Mark S. Gordon Festschrift***".

6. Chattopadhyay and co-workers have contributed **TWO** invited papers for the special issue of the ***Journal of Physical Chemistry (American Chemical Society)*** entitled ***"Structure and Dynamics: ESDMC-2013" [J. Phys. Chem. A, 117, 8555, (2013), J. Phys. Chem. A 117, 8576, (2013)].***

7. Chattopadhyay and co-workers have contributed an invited paper for the special issue of the (***Journal of Physical Chemistry (American Chemical Society)*** entitled "***Oka Festschrift: Celebrating 45 years of Astrochemistry***" ***[J. Phys. Chem. A 117, 9424, (2013)].***

8. Chattopadhyay and co-workers have contributed aninvited paper for the special issue of the ***Journal of Physical Chemistry (American Chemical Society)*** entitled ***Graham R. Fleming Festschrift [J. Phys. Chem. A 115, 3665, (2011)].***

9. Chattopadhyay and co-workers have contributed one invited article for a special issue on **"*Recent advances in electron correlation methods and applications*"** in ***Chemical Physics*(Elsevier) [*Chem. Phys. 401, 15, (2012)*] .**

10. Our paper entitled "***Taming the escape dynamics of nonadiabatic time-periodically driven quantum dissipative system within the frame of Wigner formalism***" published in ***Chemical Physics*(Elsevier) [*Chem. Phys.431*, 26 *(2014)*http://dx.doi.org/10.1016/j.chemphys.2014.01.008] was among the **10 MOST DOWNLOADED** articles in March 2014.

11. Our paper entitled "***Application of state-specific multireference Møller–Plesset perturbation theory to non-singlet states***" [***Journal of Chemical Physics (American Institute of Physics)130, 014101 (2009)***; doi:10.1063/1.3043364] was among the **20 MOST DOWNLOADED** articles in January 2009.

12. Chattopadhyay and co-workers have contributed **Two Chapters** in "***Recent Advances in Spectroscopy***: ***Theoretical, Astrophysical and Experimental Perspectives (Series: Astrophysics and Space Science Proceedings***) published by **Springer (Heidelberg, 2010).**

13. One of the figures of our paper "***State-Specific Multireference Coupled Cluster-Based Methods for Potential Energy Surfaces and Their Approximate Variants***" is the FRONT COVER IMAGE for ACS Symposium Series, Volume 828***(American Chemical Society)***: Washington, DC, edited by Hoffmann and Dyall.

Teaching:

(I) PG Teaching (Mainly Include Courses) :

1. Basic and Advanced Quantum Mechanics
2. Statistical Mechanics
3. Chemical Dynamics in Condensed Phases
4. Spectroscopy and Group Theory
5. Surface Chemistry
6. Computational Chemistry
7. Term-papers and Project Works
8. Physical Chemistry Laboratory

(II) UG Teaching (Mainly Include Courses):

(1) Chemical Kinetics
(2) Electrochemistry
(3) Phase Rules
(4) Chemistry Laboratory

Research Focus:

(I) **Electronic Structure Theory:** Current research of our group includes development and applications of computationally cost-effective size-extensive relativistic and nonrelativistic non-variational wave functions methods such as MRCC and MRPT protocols for the estimations and predictions of electronic structural properties for closed and open-shells atomic and molecular systems and metastable electronic states (resonances). In addition, we also like to develop tools for describing response properties.Our main interest is in high accuracy methods and methods based on first principles of quantum mechanics that allow us to be predictive.

(II) **Chemical dynamics in condensed phases:** Another focus of our research is the investigation the dynamics of small systems and pertinent properties. The properties of objects at the nano-scale are governed by the intricate inter-play of both thermal fluctuations and quantum effects which are moreover strongly affected by the coupling to external environments. The study of the dynamics becomes particularly rich and challenging when system and/or environment are in the influence of external rapidly oscillating forces.

Grants Support

1. **CSIR (New Delhi, 2019):** Title "Development and application of costeffective ***ab initio*** methods for strongly correlated electrons: A challenge for electronic structure theory"[Ref. No.: 01(7836)/19Effective from May 1, 2019] (Completed).

2. **DST (New Delhi, 2016)**: Title "Profiling the electronic structure properties of relativistic and non-relativistic systems using computationally cost effective *ab initio* methods" [CoI, Ref. No.: EMR/2015/000124, dated 28 July, 2017] (Completed).

3. **CSIR (New Delhi, 2014):** Title "Development and Application of the Theoryof Dynamical Systems to Problems in Condensed Phases" [Ref. No.: 01/2771/14/EMR-II dated 25.06.2014] (Completed).

4. **DST (New Delhi, 2010)**: Title "Relativistic study of the excited/ionized states of heavy atoms using coupled cluster based linear response theory" [Ref. No.: SR/S1/PC-61/2009] (Completed).

5. **CSIR (New Delhi, 2008)**: Title "Development and applications of theoretical models to study anisotropic diffusion and transport phenomena in some complex systems" [Ref. No.: 01/2257/08/EMR-II dated 01.11.2008] (Completed).

6. **DST (New Delhi, 2006)**:Title "Development and Applications of Intruder Free Multi-reference Perturbative and Non-perturbative Formalisms" [Ref. No.: SR/S1/PC-32/2005, dated 08.01.2007] (Completed).

7. **UGC(New Delhi)**: Title "Study of Dissipative Dynamics to Investigate the Transport Problem : Effects of Velocity Dependent Coupling"(Completed)

Ph. D. Students [*Awarded=15, and Ongoing=1*]

1. **Dr. Satyabrata Bhattarcharya** (Degree Awarded, Ref. No.: RPhD-1/302/11, dated 18 April, 2011, BESU, Shibpur)
2. **Dr. Pradipta Ghosh** (Degree Awarded, Ref. No.: RPhD-1/305/11, dated 18 April, 2011, BESU, Shibpur)
3. **Dr. Madhulita Das** (Degree Awarded,Ref. No.: RPhD-1/357/12, dated 20 July, 2012 , BESU, Shibpur)
4. **Dr. Anindita Shit** (Degree Awarded, Ref. No.: RPhD-1/424/13, dated 03 December, 2013, BESU, Shibpur)
5. **Dr. Prasanth Mohan**(Degree Awarded, Ref. No.: RPhD-1/449/14, dated 15 April, 2014, BESU, Shibpur)
6. **Dr. Tarunendu Mapder**(Degree Awarded, Ref. No.: RPhD-1/650/17, dated 17April, 2017, IIEST, Shibpur)
7. **Dr. Prasun Sarkar** (Degree Awarded, Ref. No.: RPhD-1/657/17, dated 25 September, 2017, IIEST, Shibpur)
8. **Dr. Suvonil Sinha Ray** (Degree Awarded, Ref. No.: RPhD-1/758/18, dated 09 October, 2018 IIEST, Shibpur)
9. **Dr. Anirban Ghosh**(Degree Awarded, Ref. No.: RPhD-1/782/18, dated 12 December, 2018 IIEST, Shibpur)
10. **Dr. Achintya Mandal,** (Degree Awarded, Ref. No.: RPhD-1/821/19, dated June 4, 2019 IIEST, Shibpur)
11. **Dr. Jagannath Das** (Degree Awarded, Ref. No.: RPhD-1/1018/21, dated August 13, 2021 IIEST, Shibpur)
12. **Dr. Shovan Manna** (Degree Awarded, Ref. No.: RPhD-1/1010/21, dated August 4, 2021 IIEST, Shibpur)
13. **Dr. Papri Mandal (**Degree Awarded, Ref. No.: RPhD-1/1131/22, dated August 16, 2022 IIEST, Shibpur)
14. **Dr. Saheli Ghosal** (Degree Awarded, Ref. No.: RPhD-1/1060/22, dated November 2, 2022 IIEST, Shibpur)

15. **Dr. Anamika Ghosh** (Degree Awarded, Ref. No.: RPhD-1/1236/23, dated December 1, 2023 IIEST, Shibpur)
16. **Mr. Rajib Adhikary** (Registered, IIEST, Shibpur)

Administrative Activities/ Institute Support Works

(I) Head of The Department, Chemistry, IIEST, SHibpur [December 2019-2022]
(II) Shodhganga, Coordinator 2022-
(III) Chairman, Library Advisory Committee, Office Order No. RDO/531/18 (dated 14/11/2018) [From 2018- Till now]
(IV) Chairman of Convocation Management Committee (2021) [Office Order No. RMS/277/21, dt. 09/6/2021].
(V) Coordinator-QIP and CEP Cell, IIEST, Shibpur [May-2015 –Till Now].
(VI) Committee member of IPR Cell, IIEST, Shibur
(VII) Member of DPGC of various Departments of IIEST, Shibpur.
(VIII) IRINS-Vidwan, Nodal Officer, IIEST, Shibpur [June-2019 –Till Now]
(IX) Convenor, Committee for Central Facility of High-End Computing, Office Order No. RC-Noti/Dean/2019/181, dated 12 February, 2019
(X) Professor-in-Charge of Dr. M. N. Dastur School of Material Sciences and Engineering from 9th March to 4th April 2019. Office order No: RDO/885/19, dated 7 March, 2019.
(XI) Chairman for the Committee constituted by the Director for framing the guidelines for conducting Conference/ Seminar / Workshop/ Faculty Development Programme and similar such programs (Office order No.: RDO/52/18, dated 06/07/2018).
(XII) Associate Dean (Academic) Office Order No. RDO/030/15 (dated 03/03/2015) [Mar-2010 –May 2018].
(XIII) Professor in-charge Library Office Order No. RDO-2/4058 (dated 29/01/2010) [Mar-2010 –Till 2018].
(XIV) Convener of Committee for "Leave rules and LTC rules of the Institute" (office order No: AT/EC/44.01.01/2014/298, dated14.07.2014).
(XV) Centre In-charge (M. Sc Admission and CCMN) [2015 –2018].
(XVI) Course Coordinator (Research Methodology) [2015 –2018].
(XVII) Test coordinator for "Student Learning Assessment (SLA) Under TEQUIP- III project of IIEST" (Office order No:2927/D(AH)/17, dated14.11.2017).
(XVIII) Convener of "Regulations for the Doctoral Programme leading to PhD degree of IIEST, Shibpur, (Office order No. RMS/6341/17, dated 23.11.2017).
(XIX) Convener of "Appeal of some research fellows to grant SRF with effect from 01.10.2014" (Office order No: RMS/6364/17, dated 23/11/17).
(XX) Convener of "Enquire committee, (office order, Office orderno.2819/D(AA)/17, dated September 22,2017).
(XXI) Convener of Committee, "5-year integrated M.Sc. Programme in basic sciences after 10+2 years of schooling (or equivalent)".
(XXII) Chairman of committee related to the loss of a number of books from CRL,

IIEST-Shibpur, (Office order No. 3/22/D(DA)/17, dated 20/12/2017).

(XXIII) Convener of Enquire Committee (Office order No. RMS-1/294, dated 23/05/2013).

List of Publications (Sudip Chattopadhyay)

Year – 2024

1. Nandi M., **Chattopadhyay, S**., Bandyopadhyay, S., and Banik, S. K. **(2024)** "Channel assisted noise propagation in a two-step cascade", **Chaos** (Under revision)

2. **Chattopadhyay, S.** and Chaudhuri, R. K. **(2024)** "Identification of the Ground State of Carbenes using DFT-based multi reference perturbative approach", ***J. Phys. A*** (**to be Communicated**).

3. **Chattopadhyay, S.** and Chaudhuri, R. K. **(2024)** "Exploration of the quasidegeneracy of varying degrees using density functional-based multireference perturbation theory: A single-root approach" ***J. Chem. Phys.*** (**to be communicated**).

Year – 2023

4. Subhra Roy, T., Nandi, M., **Chattopadhyay, S**., Chaudhuri, P. and Banik, S. K. **(2023)** "Inter-play of degeneracy and non-degeneracy in fluctuations propagation in coherent feed-forward loop motif" 093502, ***J. Stat. Mechs.***

5. Chaudhuri, R. K. and **Chattopadhyay, S. (2023)** "Geometrical structure and stability of buckminsterfullerene complexes containing mono- and poly-atomic molecules, **135**, 69, ***J. Chem. Sci.*** (Invited Article, Special Issue on Interplay of Structure and Dynamics in Reaction Pathways, Chemical Reactivity and Biological Systems).

6. Shit, A. and **Chattopadhyay, S. (2023)** "Coupled-Custer Methods for Modeling Multireference Chemistry: Recent Developments" in ***Advances in Chemistry Research,*** **J. C. Taylor (Editor)** [**Invited Article**, Chapter 6, NOVA Science Publisher, USA, 2023].

Year – 2022

7. Adhikary, R., De, A., **Chattopadhyay, S.,** and Datta, J. **(2022)** "Featured contributes of Pd-Co decorated MnO2 NPs toward ORR kinetics in low temperature fuel cell: Outstanding electro-catalysis eliminating Pt and Carbon from electrodes ***"Energy Fuels***, **36**, 14411

8. Chaudhuri, R. K. and **Chattopadhyay, S. (2022)** "Relativistic studies of electronic states of diatomic Cu, Ag, and Au-systems" ***AIP-Advances*** **12,** 125019**.**

Year – 2021

9. **Chattopadhyay, S. (2021)** **"**Single-Root Multireference Brillouin–Wigner Perturbative Approach to Excitation Energies" ***ACS Omega*** **6,** 1668−1686.

10. Chaudhuri, R. K. and **Chattopadhyay, S. (2021)** "A Fock-space coupled cluster-based probing of the single- and double-ionization profiles for the poly-cyclic aromatic hydrocarbons and conjugated polyenes" ***J. Chem. Phys***. **154**, 114106.

11. Chaudhuri, R. K. and **Chattopadhyay, S.(2021)** "Description of the Methylene Amidogene Radical and Its Anion with an Economical Treatment of Correlation Effects Using Density Functional Theory Orbitals" ***J. Phys. Chem. A*** **125**, 543−558.

Year – 2020

12. **Chattopadhyay, S. (2020) "**Investigation of Multiple Bond Dissociation Using Brillouin-Wigner Perturbation with Improved Virtual Orbitals"***J. Phys. Chem. A***124,** 1444**.**

13. Das, J., Mapder, T. , **Chattopadhyay, S.**, Banik. S. K., **(2020)**" Computational study of parameter sensitivity in DevR regulated gene expression" ***PLoS ONE*** **15(2),** e0228967

14. Manna, S., Sinha Ray, S., Ghos, P., **Chattopadhyay, S.(2020)** "Structural properties and isomerization of simple S-nitrosothiols: Ab initio studies with a simplified treatment of correlation effects" ***Mol.Phys***. **118**, e1641639.

15. Manna, S., Chaudhuri, R. K. and **Chattopadhyay, S.(2020)** "Taming the Excited States of Butadiene, Hexatriene and Octatetraene using State Specific Multireference Perturbation Theory with Density Functional Theory Orbitals" ***J. Chem. Phys*****. 152**, 244105 (2020).

16. Sharma, A., **Chattopadhyay, S**., and Sinha, D. (**2020**) "Exploring the spectroscopic constants of $^2\Pi_u$, $^2\Sigma_u^+$ Main and Satellite, and $^2\Pi_g$ states of N_2^+ ion through the window of eigenvalue independent partitioning: A Fock space coupled cluster approach" ***Mol. Phys.*** **118,** e1774673 ***[SPECIAL ISSUE OF MOLECULAR PHYSICS IN HONOUR OF JÜRGEN GAUSS]***

17. **Chattopadhyay, S. (2020)**"Perturbative Account of Electron Correlation Effects in the Internal Rotational Barrier of Molecules: A State Specific Strategy" **Series:** ***Chemistry Research and Applications,*** **Nadia T. Paulsen (Editor) [Invited Article**, Chapter 5, NOVA Science Publisher, USA, 2020].

Year – 2019

Electronic Structure Theory (Relativistic and Nonrelativistic):

18. **Chattopadhyay, S.(2019)** "Simplified Treatment of Electronic Structures of the Lowest Singlet and Triplet States of Didehydropyrazines" ***J. Phys. Chem. A, 123,*** 5980.

19. **Chattopadhyay, S.(2019)** "*Ab initio* probing of the ground state of tetraradicals: Breakdown of Hund's rule" ***J. Phys. Chem. A*123**, 2211-2226.

20. Sinha Ray, S., Manna, S., Ghosh, A., Chaudhuri, R. K., and **Chattopadhyay, S**. (**2019**) "Multireference perturbation theory with improved virtual orbitals for multiradicals: More degeneracies and more problems" ***Int. J. Quantum Chem.*119**, e25776.

21. Chaudhuri, R. K., and **Chattopadhyay, S**. (**2019**) "Fock-space multireference coupled cluster calculations of Auger energies of noble gas elements using relativistic spinors" ***J.Chem. Phys.*151, 074114.**

22. Manna, S., Sinha Ray, S.,**Chattopadhyay, S.**and Chaudhuri, R. K. **(2019)** "A simplified ministration of the correlation effects to bond breaking processes: The Brillouin-Wigner perturbation theory using a multireference formulation" ***J. Chem. Phys.*,151, 064114.**

Year – 2018

Electronic Structure Theory (Relativistic and Nonrelativistic):

23. **Chattopadhyay, S**. **(2018) "**The effect of substituents on energy splitting in organic radicals: Quantitative cognizance from *ab initio* studies", ***Chem. Phys.513***, 230–240.

24. **Chattopadhyay, S.(2018)** "Description of quasidegenerate electronic states exhibiting avoided crossing" ***Mol. Phys. 116***, 2343–2363.

25. Chaudhuri, S. K., Mukherjee, P., Chaudhuri R. K., and **Chattopadhyay, S.(2018)**"Equation of motion approach for describing allowed transitions in Ne and Al^{3+} under classical and quantum plasmas" ***Phys. Plasma*25**, 042705.

26. Manna, S., Sinha Ray, S., Ghos, P., **Chattopadhyay, S.(2018)** "On the conversion XCN ↔ XNC via an efficient and economic perturbative wavefunction approach" ***Mol. Phys. 116***, 2147–2161.

Year – 2017

Electronic Structure Theory (Relativistic and Nonrelativistic):

27. Sinha Ray, S., Manna, S., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "Description of C_2 dissociation using a naive treatment of dynamical correlation in the presence of quasidegeneracy of varying degree" **Mol. Phys.115,** 2789-2806 (**Invited**, ***Special Issue in Honor of Debashis Mukherjee***).

28. Ghosh. A., Sinha Ray, S., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "Four-Component Relativistic State-Specific Multireference Perturbation Theory with a Simplified Treatment of Static Correlation" ***J. Phys. Chem. A121***, 1487−1501(**Invited, Special Issue**"**Mark S. Gordon Festschrift**")."

29. Sinha Ray, S., Ghosh, P., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "Improved virtual orbitals in state specific multireference perturbation theory for prototypes of quasidegenerate electronic structure" **J.*Chem. Phys*.146**, 064111.

30. Sinha Ray, S., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "Communication: Viewing the ground and excited electronic structures of platinum and its ion through the window of relativistic coupled cluster method" ***J. Chem. Phys*** 146, 011102.

31. Chaudhuri, S. K., Chaudhuri R. K., Mukherjee, P. and **Chattopadhyay, S.** (2017) "A confinement induced spectroscopic study of noble gas atoms using equation of motion architecture: Encapsulation within fullerene's voids" ***J. Chem. Phys*.147**, 034111.

32. Sinha Ray, S., Ghosh, A., Shit, A., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "A simplified *ab initio* treatment of diradicaloid structures produced from stretching and breaking chemical bonds" ***Phys. Chem. Chem. Phys*.19**, 22282**.**

33. Sinha Ray, S., Mahapatra, S. U., Chaudhuri, R. K., and **Chattopadhyay, S**. (2017) "Combined complete active space configuration interaction and perturbation theory applied to conformational energy prototypes: Rotation and inversion barriers" ***Comp. Theor. Chem*.1120** 56–78.

Year – 2016

Electronic Structure Theory (Relativistic and Nonrelativistic):

34. **Chattopadhyay, S**.,Chaudhuri, R. K., Mahapatra, U. S., Ghosh, A., and Sinha Ray, S.**(2016)** "State-specific multireference perturbation theory: Development and present status" ***WIREs Comput Mol Sci*** **2016,** 266–291 **(Invited Advanced Review Article).**

35. Banerjee, D.,Mondal**,** M., **Chattopadhyay, S**.,and Mahapatra, U. S. **(2016)"**A state-specific multireference coupled cluster approach with a cost effective treatment of connected triples: Implementation to geometry optimization" **Mol. Phys.114,** 1591-1608.

36. Sinha Ray, S., Ghosh, A.,Chaudhuri, R. K., and **Chattopadhyay, S**. (2016) "Taming the Electronic Structure of Diradicals Through the Window of Computationally Cost Effective Multireference Perturbation Theory" **J. Phys. Chem. A120**, 5897−5916

37. Ghosh, A., Chaudhuri, R. K., and **Chattopadhyay, S**. (2016)"Relativistic state-specific multireference coupled cluster theory description for bond-breaking energy surfaces"**J.*Chem. Phys*.145**, 124303 (1-15).

Year – 2015

Electronic Structure Theory (Relativistic and Nonrelativistic):

38. **Chattopadhyay, S**.,Chaudhuri, R. K., and Mahapatra, U. S. (**2015)** "State-specific multireference perturbation theory with improved virtual orbitals: Revisiting the ground state of F_2, Be_2, and N_2" ***J. Com. Chem.* 36**, 907-925.

39. Mahapatra, U. S., Banerjee, D., Chaudhuri, R. K., and **Chattopadhyay, S**. (**2015)** "Profiling the binding motif between Be and Mg in the ground state via a single-reference coupled cluster method" ***Mol. Phys. 113,*** 1387-1395.

40. Sharma, A., **Chattopadhyay, S.,** Adhikari, K., and Sinha, D., **(2015)**"Spectroscopic constants relating to ionization from the strongest bonding and inner valence molecular orbital $2\sigma_g$ of N_2 : An EIP-VUMRCC search" ***Chem. Phys. Lett*.634**, 88–94

41. Ghosh, A., Chaudhuri, R. K., **Chattopadhyay, S**. and Mahapatra, U. S. (**2015)**"Relativistic state-specific multireference perturbation theory incorporating

improved virtual orbitals: Application to theground state single-bond dissociation*"**J. Com. Chem.* 36,** 1954-1972**.**

Statistical Mechanics (Equilibrium and Non- equilibrium Aspects)

42. Sarkar, P., Shit, A., **Chattopadhyay, S.**, and Banik, S. **(2015) "**Profiling the overdamped dynamics of a nonadiabatic system**"*Chem. Phys.*458,** 86–91.

43. Mapder, T., Talukdar, S., **Chattopadhyay, S.**, and Banik, S. **(2015)** "Deciphering parameter sensitivity in the BvgAS signal transduction" ***PLoS ONE*, 11(1), (2015), e0147281, doi:10.1371/journal.pone.0147281**.

Year – 2014

Electronic Structure Theory (Relativistic and Nonrelativistic):

44. Mohan, P. Mangalam, A. **Chattopadhyay, S.**, **(2014)** "Parametric models of the periodogram" ***J. Astrophysics & Astronomy*, Special Issue (Proceedings of a meeting entitled "Variability of Blazars: From Jansky to Fermi" held in Guangzhou, China, December 14–16, 2012)***Edited by* J. H. Fan, Y. Liu, A. C. Gupta, & Z. Q. Shen.

45. Mahapatra, U. S and **Chattopadhyay, S.(2014)** "Binding in Beryllium Dimer: Contingent on the effects of electron correlations" ***Science Journal***, MAC**.**

46. Chattopadhyay, S., Mahapatra, U. S. and Chaudhuri, R. K. **(2014)**"Dissociation of homonuclear diatomic halogens via Multireference coupled cluster study" ***Mol. Phys.112***, 2720**DOI:**10.1080/00268976.2014.906675

47. Banerjee, D. Ghosh., A. **Chattopadhyay, S.**, Ghosh, P. and Chaudhuri, R. K. (**2014)**"Reinvestigating the ``*cis*-effect" in 1,2-difluoro derivatives of ethylene and diazene using *ab initio*multireference method" ***Mol. Phys.*112**3206.

Statistical Mechanics (Equilibrium and Non- equilibrium Aspects)

48. Shit, A., **Chattopadhyay, S.** and Ray Chaudhuri, J. **(2014)** "Taming the escape dynamics of nonadiabatic time-periodically driven quantum dissipative system within the frame of Wigner formalism" ***Chem. Phys. 431*** 26.

49. Sarkar, P., Maity, K. A., Shit, A., **Chattopadhyay, S.,** Banik, S. K.,and Ray Chaudhuri, J. **(2014) "**Controlling mobility via rapidly oscillating time-periodic stimulus" ***Chem. Phys. Lett.* 602**, 4

Year – 2013

Electronic Structure Theory (Relativistic and Nonrelativistic):

50. K. Adhikari, **S. Chattopadhyay**, B. K. De, A. Sharma, R. K. Nath,and D. Sinha (**2013**) "Search of truncation of (N-1) electron basis containing full connected triple excitationsin computing main and satellite ionization potentials via Fock space coupled cluster approach" ***J. Comp. Chem.*** **34,** 1291**.**

51. Chaudhuri, R. K., **Chattopadhyay, S**., Freed K. F., U. S. Mahapatra (**2013)** "Theoretical studies of the ground and excited state structures of stilbene" ***J. Phys. Chem. A 117,*** *9424.****Invited Article*** in**Special Issue**: "***Oka Festschrift: Celebrating 45 Years of Astrochemistry***"

52. Chaudhuri, R. K.**Chattopadhyay, S.,** andMahapatra, U. S. **(2013), "**Taming the electronic structure of lead and eka-lead (Flerovium) by the relativistic coupled-cluster method**"*J. Phys. Chem. A* 117**, 8555. ***Invited Article in*** S**pecial Issue: "*Structure and Dynamics: ESDMC-2013*"**

53. Chaudhuri, R. K., **Chattopadhyay, S**., and Mahapatra, U. S (**2013)** "Reappraisal of nuclear quadrupole moments of atomic halogens via relativistic coupled cluster linear response theory for the ionized process" ***J. Phys. Chem. A*** **117**, 12616**.**

Statistical Mechanics (Equilibrium and Non- equilibrium Aspects)

54. Shit, A., **Chattopadhyay, S.** andRay Chaudhuri, J. **(2013)**"Kapitza-Landau time window for a periodically driven system with friction: A system-bath Hamiltonian approach*"****Eur. J. Phys. B*** **86, 23.**

55. Shit, A., **Chattopadhyay, S.** and Ray Chaudhuri, J. **(2013) "**Quantum stochastic dynamics in presence of a time-periodic rapidly oscillating potential: Nonadiabatic escape rate"***J. Phys. Chem. A*** **117**, 8576. ***Invited Article in S*****pecial Issue: "*Structure and Dynamics: ESDMC-2013*" .**

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