Dr. Debashree Ghosh
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Education

Cornell University Ithaca, NY
M.S., *Chemistry and Chemical Biology* *Aug 2005 – Dec 2007*
(Grade 3.54/4.0)
Ph.D., *Chemistry and Chemical Biology* *Sept 2009*
Advisor : Prof. Garnet K.-L. Chan; Committee Members : Prof. Roald Hoffmann, Prof. Gregory S. Ezra
Thesis title : Advances and Application of Static and Dynamic Correlation Methods in ab-initio Quantum Chemistry

Indian Institute of Science Bangalore, India
M.S., *Chemical Sciences (CGPA: 7.0/8.0)* *Aug 2002- Jul 2005*
Advisor : Prof. S. Yashonath

Presidency College (Calcutta University) Kolkata, India
B.Sc. : *Chemistry Major (Grade : 77.5%)* *1999-2002*
University Rank – 4th

Professional Experience

- **University of Southern California**, Los Angeles, CA
  Postdoctoral research associate with Prof. A. I. Krylov (Sept 2009-June 2012)
- **CSIR-National Chemical Laboratory**, Pune India
  Senior Scientist, Physical and Materials Chemistry Division (July 2012-June 2017)
- **Academy of Scientific and Innovative Research (AcSIR)**, India
  Assistant Professor (May 2013 – June 2017)
- **Indian Association for the Cultivation of Science**, Kolkata, India
  Associate Professor, School of Chemical Sciences (June 2017 – current)
- **Associate Editor, Royal Society Open Science,** Royal Society Publishing, London, (2019-2022)
- **Visiting Professor, University of Michigan**, Ann Arbor, USA (2020-2021) (Fulbright Fellow)

Honors and Fellowships

- Annual Medal of the International Academy of Quantum Molecular Science (IAQMS), 2021
- Editorial Board Member, Physical Chemistry Chemical Physics, 2020-
- Fulbright-Nehru Academic and Professional Excellence Fellowship, 2020-2021
- Physical Chemistry Chemical Physics, Emerging Investigator Lectureship Award, 2018.
- Humboldt Research Fellowship for Experienced Researchers, 2017-18.
- Carl Frederich von Siemens Fellowship, 2017-18
- Editorial Board Member, International Journal of Quantum Chemistry, 2018-
- Editorial Board Member, Electronic Structure, 2018-
- Invited Feature Article in J. Phys. Chem. A.
- WISE Merit Award for Excellence in Postdoctoral Research 2011
- ACTC postdoctoral Travel Fellowship 2011
- Burg Postdoctoral Teaching Award 2011
- Young investigator award in GRC (Radiation chemistry) 2010
- Best Poster award in WATOC 2008
- Cornell University graduate school travel grant 2008

Memberships and Professional Services

- Associate Editor, Royal Society Open Science, 2019-
- Editorial Board Member, Physical Chemistry Chemical Physics, 2020-
- Editorial Board Member, International Journal of Quantum Chemistry, 2018-
- Editorial Board Member, Electronic Structure, 2018-
- Expert Member of the Subgroup ”Materials and Computational Chemistry” at the National Supercomputing Mission, 2016-
- Referee for J. Am. Chem. Soc., J. Phys. Chem. A, J. Phys. Chem. B, Phys. Chem. Chem. Phys., Int. J. Q. Chem. and J. Chem. Sci.
- Member of American Chemical Society (2016-)
- Member of Exciting Science Group, Pune (2014-2017)

Invited Articles in Refereed Journals

- Hybrid equation of motion coupled cluster / effective fragment potential method : Route to understanding photo-processes in condensed phases, **D. Ghosh***, *J. Phys. Chem .A (Invited Feature Article and Cover page)*, **121(4)**, 741 (2017).
- Multiscale modelling : Hybrid quantum mechanics / molecular mechanics as an example and some recent developments, **D. Ghosh***, *Current Science (special issue)*, **112(7)**, 1455 (2017).
- Comparison of TDDFT and multireference treatment of ground and excited states of Fe(II) ammonia octahedral complex, K. Seth, **D. Ghosh***, *J. Ind. Chem. Soc.*, **96**, 801 (2019).

Publications

1. Radiationless decay processes of an unnatural DNA base: Pyrrole 2-carbaldehyde, P. Ghosh, A. Ghosh, **D. Ghosh***, *J. Phys. Chem. A*, **125(25)**, 5556 (2021).
2. Electron attachment to cytosine: the role of water, P. Verma, **D. Ghosh**, A. K. Dutta, *J. Phys. Chem. A*, **125(22)**, 4683 (2021).
3. Configuration Interaction trained by neural networks : Application to model polyaromatic hydrocarbons, S.K. Ghosh, M. Rano and **D. Ghosh***, *J. Chem. Phys.*, **154**, 094117 (2021). [Selected as Editor's pick and included in Special Issue in honor of Women in Physical Chemistry and Chemical Physics]
4. Effect of dimerization on the non-radiative processes of eumelanin monomer, P. Ghosh and **D. Ghosh***, *J. Phys. Chem. B*, (2021)
5. Computational Aspects towards understanding the photoprocesses in eumelanin, **D. Ghosh***, *WIRES Computational Molecular Science*, **11(3)**, e1505 (2021). [Highlighted in Advanced Science News]
6. Charge Transfer in DHICA eumelanin-like oligomers: role of hydrogen bonds, A. Chowdhury, **D. Ghosh***, *Chem. Comm.*, **56(72)**, 10481 (2020).
7. Comprehending the quadruple bonding conundrum in C_2 from excited state potential energy curves, I. Bhattacharjee, **D. Ghosh***, A. Paul*, *Chemical Science*, **11**, 7009 (2020). [ChemSci Pick of the week and Hot article of the year, highlighted in chemistry world]
8. Support vector regression based monte carlo simulation of flexible water clusters, S. Bose, S. Chakrabarty*, **D. Ghosh***, *ACS Omega*, **5(13)**, 7065 (2020).
9. Light Induced Excited Spin State Trapping in Spin Crossover Model System, S. Karmakar, **D. Ghosh**, T. Saha-Dasgupta, *Int. J. Quant. Chem.*, **120(6)**, e26122 (2020).
10. In the quest for a stable triplet state in small polyaromatic hydrocarbons : an in silico tool for rational design and prediction, M. Rano, S. K. Ghosh, **D. Ghosh***, *Chemical Science*, **10**, 9270 (2019).
11. Effect of microsolvation on the nonradiative decay of eumelanin monomer, P. Ghosh, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **21**, 26123 (2019).
12. Non-radiative decay of an eumelanin monomer : to be or not to be planar, P. Ghosh, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **21**, 6635 (2019).
13. Machine learning prediction of interaction energies in rigid water clusters, S. Bose, D. Dhawan, S. Nandi, R.R. Sarkar, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **20(35)**, 22987 (2018).
14. Evolutionary algorithm based configuration interaction approach, R. Chakraborty, **D. Ghosh***, *Int. J. Quant. Chem.*, **118(6)**, e25509 (2018).
15. Effect of solvation on the ionization of guanine nucleotide- a hybrid QM/EFP study, R. Chakraborty, S. Bose, **D. Ghosh***, *J. Comput. Chem.* , **38(29)**, 2528 (2017).
16. Unprecedented solvent induced inter-conversion between monomeric and dimeric silylene-zinc iodide adducts, S. Yadav, E. Sangtani, D. Dhawan, R. G. Gonnade, **D. Ghosh**,* S. S. Sen*, *Dalton Trans.*, **46**, 11418 (2017) .

17. Unraveling the mystery behind the observation of strong selenium hydrogen bond, K. K. Mishra, S. K. Singh, P. Ghosh, **D. Ghosh***, A. Das*, *Phys. Chem. Chem. Phys.*, **19**, 24179 (2017).
18. An Interaction Energy Driven Biased Sampling Technique: A Faster Route to Ionization Spectra in Condensed Phase, S. Bose**, D. Ghosh***, *J. Comput. Chem.* , **38(26)**, 2248 (2017).
19. Elucidating the Photoprotection Mechanism of Eumelanin Monomers, P. Ghosh, **D. Ghosh***, *J. Phys. Chem. B*, **121(24)**, 5988 (2017).
20. Electrostatic Origin of the Red Solvatochromic Shift of DFHBDI in RNA, S. Bose, S. Chkrabarty, **D. Ghosh***, *J. Phys. Chem. B*, **121(18)**, 4790 (2017).
21. The Extension of the Effective Fragment Potential Method to Macromolecules; P. Gurunathan, A. Acharya, **D. Ghosh**, D. Kosenkov, I. Kaliman, Y. Shao, A.I. Krylov, L.V. Slipchenko, *J. Phys. Chem. B*, **120**, 6562 (2016).
22. Effect of Solvation on Electron Detachment and Excitation Energies of a GFP Chromophore Variant; S. Bose, S. Chakrabarty, **D. Ghosh***, *J. Phys. Chem. B*, **120**, 4410 (2016).
23. Effect of sequence on the ionization of guanine in DNA; R. Chakraborty, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **18**, 6526 (2016).
24. Effects of the Benzoxazole Group on Green Fluorescent Protein Chromophore Crystal Structure and Solid State Photophysics; A. Ghodbane, W. B. Fellows, J. R. Bright, **D. Ghosh**, N. Saffon, L. M. Tolbert, S. Fery-Forgues, K. M. Solntsev, *J. Materials Chem. C*, **4**, 2793 (2016). [selected as "2016 Hot Topic paper"]
25. Feasibility of Ionization-Mediated Pathway for Ultraviolet-Induced Melanin Damage; M. Mandal, T. Das, B. K. Grewal, **D. Ghosh***, *J. Phys. Chem. B*, **119**, 13288 (2015).
26. Singlet-triplet gaps in polyacenes : a delicate balance between dynamic and static correlations investigated by spin-flip methods; C. U. Ibeji, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **17**, 9849 (2015).
27. Spectroscopic and Ab-Initio Investigation of 2,6-Difluorophenylacetylene-Amine Complexes: Coexistence of CH–N and Lone-Pair–pi Complexes and Intermolecular Columbic Decay; S. I. Mondal, A. Dey, S. Sen, G. N. Patwari, **D. Ghosh***, *Phys. Chem. Chem. Phys.*, **17**, 434, (2015).
28. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package; Y. Shao et al, *Mol. Phys.*, **113**, 184, (2015).
29. Electrostatics Determine Vibrational Frequency Shifts in Hydrogen Bonded Complexes!; A. Dey, S. I. Mondal, S. Sen, **D. Ghosh***, G Naresh Patwari, *Phys. Chem. Chem. Phys. (Comm)*, **16**, 25247, (2014).
30. Ionization induced tautomerization in cytosine and the effect of solvation; T. Das, **D. Ghosh***,*J. Phys. Chem. A*, **118(28)**, 5323, (2014).
31. Perturbative approximations to hybrid equation of motion coupled cluster / effective fragment potential method; **D. Ghosh***, *J. Chem. Phys.*, **140**, 094101, (2014).
32. Perturbative approximations to single and double spin flip equation of motion coupled cluster singles doubles methods; A. K. Dutta, S. Pal, **D. Ghosh***, *J. Chem. Phys.*, **139**, 124116, (2013).
33. Effective Fragment Potential method in Q-Chem electronic structure package; **D. Ghosh**, D. Kosenkov, V. Vanovschi, L. V. Slipchenko, A. I. Krylov, *J. Comput. Chem.* , **34**, 1060, (2013).

34. Towards understanding the redox properties of model chromophores from the green fluorescent protein family: An interplay between conjugation, resonance stabilization, and solvent effects; **D. Ghosh**, A. Acharya, S. Tiwari, A. I. Krylov,*J. Phys. Chem. B*, **116**, 12398, (2012).
35. First-Principle Protocol for Calculating Ionization Energies and Redox Potentials of Solvated Molecules and Ions: Theory and Application to Aqueous Phenol and Phenolate; **D. Ghosh**, A. Roy, R. Seidel, B. Winter, S. Bradforth, A. I. Krylov, *J. Phys. Chem. B*, **116**, 7269 (2012).
36. A VUV Photoionization and Theoretical Determination of the Ionization Energy of a Gas Phase Sugar (Deoxyribose); **D. Ghosh**, A. Golan, L. Takahashi, A. I. Krylov, M. Ahmed, *J. Phys. Chem. Lett.* **3**, 97 (2012).
37. Correction to What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?; K. M. Solntsev, **D. Ghosh**, A. Amador, M. Josowicz, A. I. Krylov, *J. Phys. Chem. Lett.*, **2**, 2695 (2011).
38. What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?; K. M. Solntsev, **D. Ghosh**, A. Amador, M. Josowicz, A. I. Krylov, *J. Phys. Chem. Lett.*, **2**, 2593 (2011).
39. The Effect of Solvation on Vertical Ionization Energy of Thymine: from Microhydration to Bulk; **D. Ghosh**, O. Isayev, L. V. Slipchenko, A. I. Krylov, *J. Phys. Chem. A*, **115 (23)**, 6028 (2011).
40. Non-covalent Interactions in Large Systems Described by the Effective Fragment Potential Method; **D. Ghosh**, D. Kosenkov, V. Vanovschi, C. F. Williams, J. M. Herbert, M. S. Gordon, M. W. Schmidt, L. V. Slipchenko, A. I. Krylov, *J. Phys. Chem. A*, **114 (48)**, 12739 (2010).
41. Accelerating Convergence in Iterative Solution for Large Complete Active Space Self-consistent Field; T. Yanai, Y. Kurashige, **D. Ghosh**, G. K.-L. Chan, *Int. J. Quant. Chem.*, **109 (10)**, 2178 (2009).
42. A Study of Cumulant Approximations to N-electron Valence Multireference Perturbation Theory; D. Zgid, **D. Ghosh**, E. Neuscamman, G. K.-L. Chan, *J. Chem. Phys.*, **130 (19)**, 194107 (2009).
43. Orbital Optimization in the Density Matrix Renormalization Group, with Applications to Polyenes and beta-carotene; **D. Ghosh**, J. Hachmann, T. Yanai, G. K.-L. Chan, *J. Chem. Phys.*, **128 (14)**, 144117 (2008).
44. An Introduction to the Density Matrix Renormalization Group Ansatz in Quantum Chemistry; G. K.-L. Chan, J. J. Dorando, **D. Ghosh**, J. Hachmann, E. Neuscamman, H. Wang, T. Yanai, *Prog. Theor. Chem. and Phys.*, **18**, 49 (2008).
45. Sorbates in Carbon Nanotubes: Transition from Diffusive to Super-diffusive Motion; S. Y. Bhide, **D. Ghosh**, S. Yashonath, G. Ananthakrishna, *Current Science*, **87 (7)**, 971 (2004).

Invited Talks

1. Quest for a stable triplet state in small polyaromatic hydrocarbons, Asian Photochemistry Coneference 2021, Seoul Korea (VIRTUAL)
2. Artificial neural network based configuration interaction, IUPAC, CCCE 2021 – 104th Canadian Chemistry Conference and Exhibition, Canada (VIRTUAL)

3. Artificial neural network based configuration interaction, TSRC Workshop on “New Frontiers in Electron Correlation” (VIRTUAL) 2021, Telluride USA
4. RSC-IISER Desktop Seminar with PCCP, Tiruvananthapuram, 2021 (VIRTUAL)
5. Departmental seminar, IISER Tirupati (VIRTUAL)
6. Innovation and Advances in Chemical Sciences-2, IACS, Kolkata
7. 57th Annual Convention of Chemists, Indian Chemical Society, 2020 (VIRTUAL)
8. TACC2020, Hokkaido University, Sapporo, Japan
9. WATOC2020, Vancouver, Canada
10. TSRC Workshop 2020, Telluride, USA (VIRTUAL)
11. Quest for a stable triplet state in small polyaromatic hydrocarbons, YIMQCMT, SNBNCBS Kolkata 2019
12. Machine learning in force fields and strong correlation, ML4Science, Hyderabad, India 2019
13. Singlet triplet gaps in polyaromatic hydrocarbons – effect of spin frustration and topology, Indo French Symposium on Small Molecule Activation for Fuels and Commodity Chemicals Production, IACS Kolkata 2019
14. Density Matrix Renormalization Group Study of Singlet Triplet gaps in polyaromatic hydrocarbons, APATCC, Sydney, Australia 2019
15. Photoprocesses in biological systems : Need for hybrid QM/MM with polarization, ISTCP, Tromso, Norway 2019
16. Density Matrix Renormalization Group Study of Singlet Triplet gaps in polyaromatic hydrocarbons, New Frontiers in Electron Correlation, Telluride, USA 2019
17. Photoprotection and nonradiative decay in eumelanin, IIT Bombay Diamond Jubilee Symposium, 2019
18. Spin frustration in Singlet triplet gaps of polyaromatic hydrocarbons, SDMC, Shimla, 2019
19. Photo-processes in biological systems : Need for hybrid QM/MM with polarization, Zernike institute of advanced materials, Groningen University, Netherlands, 2018
20. Self consistency free polarizable force field, TSRC Workshop, Telluride, USA, 2018
21. Self consistency free polarizable force field, ICQC, Menton, France, 2018
22. Importance of polarization for excited states of biological systems, RAMOLs, Bangalore, India, 2018
23. Machine learning polarizable force field, IACS-CESSD, Kolkata 2018.
24. Stochastic algorithms for strongly correlated systems, APCTCC, Mumbai 2017.
25. Hybrid QM/MM for biological systems, NISER, Bhubaneswar 2017.
26. Photoprotection Mechanism in Eumelanin, WATOC, Munich 2017.
27. Hybrid QM/MM for biological systems : Need for multireference, LMU Munich 2017.
28. Strongly Correlated Systems in Condensed Phases, Kaleidoscope, Goa 2017.
29. Photophysics of eumelanin, Spectroscopy and Dynamics of Molecules and Clusters, Pondicherry 2017.
30. Renormalization and evolutionary algorithms towards configuration interaction approach, Recent Advanced in many Electron Theory, Goa 2017.
31. Renormalization and evolutionary algorithms towards configuration interaction approach Theoretical Chemistry Symposium, Hyderabad, 2016.

32. Hybrid equation of motion coupled cluster / effective fragment potential as a route to excited state properties, IXth Congress of International Society for Theoretical Chemical Physics, Grand Forks, USA, 2016.
33. Spin flip equation of motion coupled cluster - a route to understand singlet fission Spectroscopy and Dynamics of Molecules and Clusters, Nainital 2015.
34. Perturbative approximations to spin flip coupled cluster and hybrid formalism with effective fragment potential, Tata Institute of Fundamental Research, Bombay (2014).
35. Recent Developments in Effective Fragment Potential, Q-Chem Developer's Meet, Berkeley (2014).
36. Hybrid QM/MM with effective fragment potential, USC 2014.
37. Recent Developments in Effective Fragment Potential, Kaleidoscope, Goa (2014).
38. Lower scaling multireference methods and its hybrid framework for excited states of systems in condensed phases, IIT Bombay 2013.
39. Perturbative approximations to spin flip coupled cluster and hybrid formalism with effective fragment potential, Recent Advances in Correlation Problem, Kolkata (2013).
40. Effective Fragment Potential: Hybrid method to accurately calculate ionization potential, redox potential and its extension to large biological systems, Indian Association for the cultivation of science, Kolkata (2013).
41. Effective Fragment Potential - extension to protein environments, Theoretical Chemistry Symposium, Guwahati 2012.
42. Understanding electron transfer processes in complex environment - Hybrid QM/EFP approach, Purdue University, West Lafayette (2011).
43. Effective Fragment Potential: Applications to ionization energy, redox potential and beyond, Lawrence Berkeley National Laboratory, Berkeley (2011).

Teaching Experience

1. Learning Chemistry with Computers, UG course, Spring 2020, 2021
2. Computer Lab and Numerical Methods, Fall 2019, 2020
3. Chemical Bonding and Electronic Structure, Fall 2019, 2020
4. Electronic Structure and Properties of Solids, Spring 2019.
5. Advanced Quantum Chemistry, IACS, Spring 2018 & Spring 2019.
6. C++ programming, SMCS, IACS, Fall 2018
7. Lecture Series on algorithms in quantum chemistry, Kurukshetra University
8. NCL211 Advanced Quantum Mechanics, Spring 2016.
9. NCL103 Basic Mathematics and Numerical Methods, Spring 2014, Spring 2015, Spring 2016.
10. NCL306 Mathematical methods, Fall 2013, Fall 2015.
11. Outreach talk on "How do computers work?" organized by Exciting Science Group to local schools.
12. Team teaching Chem 115b (advanced general chemistry for freshmen), Spring 2011, Department of Chemistry, University of Southern California.
13. Teaching assistant for 4 semesters in Chemistry and Chemical Biology, Cornell University: General Chemistry for Engineers, Physical Chemistry I and II.
14. Grading: Graduate quantum mechanics I, Graduate Mathematical Methods.

15. Classes: Teaching C++ class, Hartree Fock and few quantum chemical methods in Chan group.
16. Participated in CCMR (Cornell) Outreach Program teaching elementary school students.
17. Participated in CCMR (Cornell) Outreach Program working in development of experiments with middle school teachers.

Students Trained

- Master's Thesis : 1 Completed – Ms Avani Khadilkar (currently PhD student at Iowa state University)
- PhD Thesis : 2 completed, 7 in progress
    - Dr. Samik Bose (2020)
    - Ms. Paulami Ghosh (thesis submitted, 2021)
    - Ms. Madhumita Rano (4th year)
    - Mr. Sumanta Kumar Ghosh (3rd year)
    - Mr. Koushik Seth (3rd year)
    - Mr. Arpan Chowdhury (2nd year)
    - Ms. Tanima Kundu (1st year)
    - Ms. Mandira Dey (1st year)
    - Mr. Supriyo Santra (1st year, joint with Prof. Ankan Paul)
- Institute postdoctoral fellow and NPDF : 1 Completed - Dr. Arpita Ghosh (2019-2021)
- CSIR Nehru postdoctoral fellow : 1 Completed – Dr. Baljinder K. Grewal (2014-16)

Grants

- National Supercomputing Mission (NSM), Multireference methods with hybrid QM/MM approaches – 91.9 lakhs (2019-2022)
- DST SERB Extramural grant, Mechanism of photoprotection and photodamage in melanin and the role of heterogeneity – 46.7 lakhs (2018-2021)
- DAE-BRNS, Development of hybrid QM/MM methodologies based on effective fragment potential (EFP) – 25 lakhs (2015-2018)
- DST SERB Fast Track grant, Effect of base pairing, stacking, sequence and environment on the nature of excited states in DNA – 25 lakhs (2014-2017)