

Name: Dr. Sanghamitra Das (SD)

M.Sc., PhD

Department: Physics

Designation: Assistant Professor

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Research Interest: Quantum Many Body Methods, Non-Conventional Energy Sources



Academic Record :

- B.Sc. (Physics Hons), Lady Brabourne College (1999)
- M.Sc. (Physics), Calcutta University (2001); Specialization in High Energy Physics
- CSIR-NET (JRF) in 2001
- Ph.D. (2008), Indian Association for the Cultivation of Science; Dissertation *Applications of Molecular Many-Body Methods for Treating Strongly Correlated Molecular States*

Positions held :

- Research Associate, Budapest University of Technology and Economics, Hungary (October 2008 – September 2010)
- Research Associate, Dept. of Materials Science, IACS, Kolkata, (November 2010 – December 2010)
- Assistant Professor (Against Leave Vacancy), Dept of Physics, St. Xavier's College (Autonomous), Kolkata (January 2011 – June 2014)
- Assistant Professor (on Contract) Dept. of Physics, St. Xavier's College (Autonomous), Kolkata (July, 2014 – April, 2015)
- Assistant Professor, Dept. of Physics, Basirhat College, Basirhat (April, 2015 – July, 2017)
- Assistant Professor, Dept. of Physics, St. Xavier's College (Autonomous), Kolkata (July, 2017 - present)

Awards and Distinctions

- **State Merit Certificate** in the Madhyamik Examination of West Bengal Board of Secondary Education in 1994.
- **National Scholarship** in Physics Honors in the B.Sc. (Honors) Examination of Calcutta University in 1999.
- **Junior Research Fellowship** from **Council of Scientific and Industrial Research (CSIR)** (2002-2004)
- **Senior Research Fellowship** from **Council of Scientific and Industrial Research (CSIR)** (2004-2007)
- **Senior Research Fellowship** from **Department of Science and Technology (DST)** (2007-2008)

Membership of Professional bodies

- Life Member, Indian Science Congress

List of publications

A. Research Papers in Journals :

1. "State-specific Multi-reference Many-body Approach using Incomplete Model Spaces"; D. Pahari, S. Chattopadhyay, S. Das, D. Mukherjee, Chem. Phys. Lett. 381, 223 (2003).
2. "An Externally-corrected size-extensive single-root MRCC formalism: Its kinship with the rigorously size-extensive state-specific MRCC theory"; S. Das, N. Bera, S. Ghosh and D. Mukherjee, Theor. Chim. Acta. 771, 79 (2006).
3. "Development and pilot molecular applications of the uncoupled state-specific MRCC(UC-SS-MRCC) theory" S. Das, D. Datta, R. Maitra and D. Mukherjee, Chem. Phys. 349, 115 (2008).
4. "Effective $\frac{1}{4}$ -electron Hamiltonian for small-radius nanotubes: Interpretation of curvature-induced conductivity"; P. Szakacs, P. R. Surjan, D. Mukherjee and S. Das, Phys. Rev. B 77, 193407 (2008).
5. "Comparative study of multi-reference perturbative theories for ground and excited states"; M. R. Hoffmann, D. Datta, S. Das, D. Mukherjee, A. Szabados, Z. Rolik, P. R. Surjan; J. Chem. Phys. 131, 204104 (2009).
6. "Full implementation and benchmark studies of Mukherjee's state-specific multireference coupled-cluster ansatz"; S. Das, D. Mukherjee and M. K'allay; J. Chem. Phys. 132, 074103 (2010)
7. "High-accuracy Thermochemistry of Atmospherically Important Fluorinated and Chlorinated Methane Derivatives"; J. Csontos, Z. Rolik, S. Das, M. K'allay; J. Phys. Chem. A. 114, 13093 (2010)
8. "Inclusion of Selected Higher Excitations involving Active orbitals in the State-specific Multi-reference Coupled-Cluster Theory"; S. Das, M. K'allay, D. Mukherjee; J. Chem. Phys. 133, 234110 (2010)
9. "High-accuracy theoretical thermochemistry of atmospherically important nitrogen oxide derivatives"; P. Szakacs, J. Csontos, S. Das, M. K'allay; J. Chem. Phys. A. 115, 3144 (2011)
10. "Superior Performance of Mukherjee's State-specific Multi-reference Coupled-Cluster Theory at the Singles and Doubles Truncation Scheme with Localized Active Orbitals"; S. Das, M. K'allay, D. Mukherjee; Chem. Phys. (in press, Accepted Manuscript)

B. Book Chapters :

11. Size-consistent State-specific Multi-reference Methods: A Survey of Some Recent Development: D. Pahari, S. K. Chattopadhyay, S. Das, D. Mukherjee and U. S. Mahapatra; in First 40 years of Quantum Chemistry, Ed: C. E. Dykstra, K. S. Kim, G. Frenkin, and G. E. Scuseria (Elsevier 2005)
12. Development and Applications of Non-Perturbative Approximants to the State-specific Multi-reference Coupled Cluster Theory: The Two Distinct variants: S. Das, S. Pathak, R. Maitra and D. Mukherjee; in Recent Progress in the Coupled Cluster Theory and Applications Series: Challenges and Advances in Computational Chemistry and Physics, Vol. 11, Ed: P. Carsky, J. Paldus, J. Pittner (Springer 2010) pp.-57