Dr. Sanghamitra Das

Department: Physics

Qualification : M.Sc., Ph.D.

Designation: Assistant Professor

Publications in Journals:

(i) ”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).

(ii) ”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).

(iii) ”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).

(iv) ”ı1Effective ¼-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).

(v) ”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. Surj´an;
J. Chem. Phys. 131, 204104 (2009).

(vi) ”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)

(vii) ”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)

(viii) ”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)

(ix) ”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)

(x) ” 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)

Publications in Books:

(i) 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)

(ii) 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