DEBASIS JANA

HOD & Associate Professor, Department of Chemistry

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Academic Background

Ph. D. work at **IACS (1995-2001)** and degree awarded from **Jadavpur University in 2002.**

M.Sc. Chemistry, **IIT Kanpur (1995)**

B.Sc. Chemistry (Hons) **Presidency College, Kolkata (1993)**

Teaching Areas

o   Theoretical Physical Chemistry (Mainly includes - Classical Thermodynamics/Quantum Chemistry/Fundamental Statistical Thermodynamics/Solid State Structure in Chemistry)

o   Laboratory Experiments based on Physical Chemistry for UG as well as PG courses (Applied Chemistry)

o   Basic Computer Programming in Fortran language

Teaching Experience

✓   BSc, RKM Vidyamandira

✓   MSc, RKM Vidyamandira

✓   MSc, RKM Residential College

✓   Training for Chemistry Olympiad, HBCSE

✓   MSc, Asutosh College (IGNOU)

Research Interests

•   *Study of core and core-valence correlation and relaxation in strongly correlated systems*

•   *Study of orbital-localization for molecular systems with heavy atoms*

Research Experience

➕   *Open-shell Fock-space Coupled Cluster Theory* [Ph.D. work, **Department of Physical Chemistry, IACS, Kolkata,** with **Prof. Debashis Mukherjee]**

➕   **Ph.D. thesis -** *Development and Applications of Many-body methods for Orbital relaxation and Differential correlation effects* – **IACS (2002)**

➕   *A theoretical study of solvation dynamics in electrolyte solutions* – IIT Kanpur (1995)

➕   *Purification of Yeast hexokinase and effect of phosphate on enzyme activity* – TIFR, Mumbai (1994)

Projects Completed

➢   Minor Research Project (UGC) [PSW-043/08-09 (ERO)] - *Many-body approach to study the properties of strongly correlated systems – ionized /excited states*

➢ Minor Research Project (UGC) [PSW-108/15-16 (ERO)] – *Study of core and core-valence correlation and relaxation in multi-valence problem using many-body approach*

- *A compact spin-free MRCC theory for the state energy per se* (**Poster**) – **52nd ANNUAL CONVENTION OF CHEMISTS 2015 and International Conference on Recent Advances in Chemical Sciences** organized by **Indian Chemical Society** at **JECRC University**

- *Study of Possible symmetry Breaking in Core Holes – A relaxation based valence MRCC approach* (**Poster**) – **52nd ANNUAL CONVENTION OF CHEMISTS 2015 and International Conference on Recent Advances in Chemical Sciences** organized by **Indian Chemical Society** at **JECRC University**

- *A fully connected relaxation-based MRCC theory for the state energy per se* (**Poster**) – **National Symposium on Facets of Chemistry in Biology FOCB-2016** organized by **St. Xaviers' College**

- *A strongly connected Relaxation-based Valence-specific theory for ionized states* (**Poster**) – **National Seminar on Current Trends in Chemistry VII** (2016) at **Kalyani University**

Students Working with

Aakash Gupta, UG 3rd yr, *Schottky defects in crystals and statistical calculation, (*Since 2019) [Participated in International symposium, organized by Ind Chem Soc, Dec'20 and awarded as one of four best posters]

Kunal Chowdhury, UG 2nd yr, *Need of Equations in Modern Periodic table* (Since 2020) [Participated in International symposium, organized by Ind Chem Soc, Aug'21]

Research Publications

1. Controllable white light generation from novel $BaWO_4$: Yb^{3+}/Ho^{3+}/Tm^{3+} nanophosphor by modulating sensitizer ion concentration, Bibek Samanta, Arnab Kumar Dey, Preetam Bhaumik, Sumanta Manna, Anupam Halder, **Debasis Jana,** Kalyan K. Chattopadhyay, Uttam Kumar Ghorai, *Journal of Materials Science: Materials in Electronics* **30**, 1068, (2019)

2. A novel VU-MRCC formalism for the simultaneous treatment of strong relaxation and correlation effects with applications to electron affinity of neutral radicals, **D. Jana**, D. Datta and D. Mukherjee, *Chem. Phys.* **329**, 290, (2006)

3. Development of a relaxation-inducing cluster expansion formalism for treating strong relaxation and correlation effects, **D. Jana** and D. Mukherjee, *J. Chem. Phys.* **122**, 234101, (2005)

4. Full effect of triples in a valence universal multi-reference coupled cluster calculation, S. Chattopadhyay, A. Mitra, **D. Jana,** P. Ghosh and D. Sinha, *Chem. Phys. Lett.* **361,** 298, (2002)

5. State-specific multi-reference perturbation theories with relaxed coefficients: Molecular applications, P. Ghosh, S. Chattopadhyay, **D. Jana** and D. Mukherjee, *Int. J. Mol. Sc.* **3**, 733, (2002)

6. Use of a new cluster Ansatz to treat strong relaxation and correlation effects: A direct method for energy differences, **D. Jana**, U. Sinha Mahapatra and D. Mukherjee, *Int. J. Mol. Sc.* **3**, 550, (2002)

7. A compact spin-free cluster expansion formalism for simple open-shell configurations, **D. Jana**, U. Sinha Mahapatra and D. Mukherjee, *Chem. Phys. Lett.* **353**, 100, (2002)

8. Development and applications of a relaxation-inducing cluster expansion theory for treating strong relaxation and differential correlation effects, **D. Jana**, B. Bandyopadhyay and D. Mukherjee, *Theo. Chem. Acc.* **102**, 317, (1999)

9. A molecular theory of frequency and wave-vector dependent dynamic response functions of electrolyte solutions, A. Chandra, **D. Jana** and S. Bhattacharjee, *J. Chem. Phys.* **104**, 8662, (1996)

Awards & Honors

o *CSIR JRF Fellowship (1995)*

o *VSRP Summer Research Fellowship (1994)*

o *WB Govt (Calcutta University National Scholarship (1993)*

Association & Membership

➕ **Member** of **Board of Studies** of **Department of Chemistry, RKMV**

➕ Member, Selection Committee, JBNSTS Fellowship, Since 2012

➕ Life Member, Indian Association for the Cultivation of Science, Since 2001

➕ Member, **Committee for New Undergraduate Syllabus for Indian Universities and Colleges (CBCS), 2016-17**

➕ Past Member, InChO, HBCSE, 2012-13

Organizing Capacity

❖ **Co-ordinator**, International Webinar on '*Chemistry in the eyes of Past and Present Vidyamandira Students*', June 2021

❖ **Jt. Convenor**, National Webinar on *'Modern Trends in Chemical Research: A few Glimpses'*, RKMV, January 2021

❖ **Co-ordinator**, National Seminar on '*Chemistry Education and Research in Daily Life*', RKMV, 2017

❖ **Co-ordinator**, National Seminar on '*CHEMSEM – 2009'*, RKMV

❖ National Seminar on '*Science Day Celebration – 2004'*, RKMV

Academic Publication

Editor, *Chemistry Comm, A Platinum Jubilee Commemorative Volume in Chemistry*, **RKMV, August 2017**

Abstracts of Selective Papers

- A novel VU-MRCC formalism for the simultaneous treatment of strong relaxation and correlation effects with applications to electron affinity of neutral radicals [*Authors*: **Debasis Jana**, Dipayan Datta and Debashis Mukherjee] **Chemical Physics 329**, 290, (2006) (Dedicated paper to Prof. L. Cederbaum on the happy occasion of his reaching 60) –

  We present and implement in this paper a novel spin-free valence-universal multi-reference coupled cluster (VU-MRCC) formalism for energy differences, which can capture orbital relaxation and correlation relaxation to all orders. Unlike in the traditional normal ordered cluster Ansatz for computing energy differences, this cluster expansion formalism allows contractions between various valence excitation operators with valence spectator lines. These contractions simulate the orbital relaxation and correlation relaxation effects for the ionized/excited states via Thouless-like exponential type of operators. Generally such operators are non-commuting. To ensure that each distinct excitation generated by contracted composites formed by these operators appear only once in the wave-operators, the factors accompanying these composites have to be judiciously chosen. Hence, the combinatoric factors accompanying such contracted composites are not taken to be 1/n! for nth-power, but rather the inverse of the automorphic factor (the number of ways the n operators can be connected in various permutations generating the same composite). It is shown that this Ansatz leads to a set of VU-MRCC equations for the valence cluster

amplitudes, in which all the cluster operators are attached to the hamiltonian by at least one non-spectator line (a strongly connected series). The series is thus terminating at the quartic power. Illustrative applications are presented by computing electron affinity of neutral doublet radicals (viz., NH2, OH, F, BO and CN), where the orbital relaxation effect attendant on the anion formation is considerable. Several basis-sets capable of describing the anions have been studied. It has been found that aug-cc-pVTZ basis gives the best overall results, while aug-cc-pVQZ overestimates the electron affinity, presumably because of an imbalance in describing the neutral radicals. The method performs consistently much better then the one with the traditional normal ordered Ansatz.

- Development of a Relaxation-inducing Cluster Expansion Formalism for Treating Strong Relaxation and Correlation Effects [*Authors*: **Debasis Jana** and Debashis Mukherjee] **Journal of Chemical Physics 122**, 234101, (2005) (Dedicated to Professor S. Hirao on the happy occasion of his reaching sixty) -

We present in this paper a comprehensive account of an explicitly spin-free coupled cluster theory for treating energy differences of open-shell states relative to a closed-shell ground state, where the open-shell states of interest are dominated by a few simple configuration state functions (CSF). We develop a valence-universal coupled cluster formalism to achieve this via a novel cluster expansion Ansatz for the valence part of the wave-operator, where the orbital relaxation and the correlation relaxation accompanying ionization/excitation from the ground state is taken care of to all orders in compact, efficient and explicitly spin-free manner. The essential difference of our proposed Ansatz from the ordinary and the normal ordered cluster Ansatz in vogue is that (a) we allow the valence cluster operators to be connected among themselves with spectator valence lines only and (b) we use suitable combinatoric factors accompanying powers of cluster operators thus connected, which are equal to the number of ways the operators can be joined, leading to the same excitation (the automorphic factor). We emphasize that such an Ansatz does not generate terms (diagrams) with chains of cluster operators joined among themselves via spectator lines only. Barring only a few, almost all the terms in the working equations determining the cluster amplitudes involve contraction of the hamiltonian with the cluster operators via at least one non-spectator line, leading to what we call a 'strongly connected' series. The structure of the working equation is remarkably similar to the single reference closed-shell equation, with a few additional terms. The presence of contractions among cluster operators via spectator lines, introduce the additional physical effects of orbital and correlation relaxation using low-body cluster operators. As an illustrative application of the new MRCC theory, we consider in this paper computation of ionization potentials (IPs) of one valence problem with only one active orbital. The numerical applications are made for both the core and the inner and outer valence IPs for several molecular systems. The numerical values demonstrate the superiority of the relaxation-inducing CC theory, as compared to the normal-ordered Ansatz.

- Use of a New Cluster Ansatz to Treat Strong Relaxation and Correlation Effects: A Direct Method for Energy Differences [*Authors*: **Debasis Jana**,Uttam Sinha Mahapatra and Debashis Mukherjee] **International Journal of Molecular Science 3**, 550 -569, (2002)

We have presented in this paper a new cluster Ansatz for the wave operator for open-shell and/or quasidegenerate states, which takes care of strong relaxation and correlation effects in a compact and efficient manner. This Ansatz allows contraction among the various cluster operators via spectator orbitals, accompanied by suitable combinatorial factors. Since both the orbital and the correlation relaxations are treated on the same footing, it allows us to develop a very useful direct method for energy differences for open shell states relative to a closed-shell ground state, where the total charge for the two states may differ. We have discussed a new spin-free coupled cluster (CC) based direct method and illustrated its performance by evaluating electron affinity of a neutral doublet radical. We have also indicated how the scope of the theory can be extended to compute the state energies of simple open shell configurations as well. In that case, the CC equations terminate after the quartic power of cluster operators exactly as in the closed-shell situation, which is not the case for the current methods.