Dr. Rajendra Saha

Designation: Associate Professor
Qualifications: M.Sc. Ph.D.

➢ B. Sc. (Hons. in Chemistry), Calcutta University, 1997.

➢ M. Sc., IIT Kanpur, 1999.

➢ Ph. D. (Chemical Science), Indian Association for the cultivation of Science, Jadavpur, 2007

Thesis Title:
"Development of Soft-Computing techniques for molecular electronic structure calculations and exploration of complex potential energy landscapes of clusters"

About Me:

- **Experience / Expertise:**

  - **Soft-Computing techniques for molecular electronic structure calculations**: Development of Genetic Algotithm (**GA**) based recipe for direct solution of Schrodinger equation for the ground and excited states of atoms and molecules with few electrons
  - **Application of GA as global optimizer**: GA used to find the global and local minimum of the potential energy landscape of the clusters of atoms, molecules, ions and their hydrates and simulation of their properties carried out using standard semi-empirical and ab-initio methods
  - **Parallelization of the GA code**: single population master-slave parallel GA implemented using MPI protocol on parallel linux-based cluster
  - **Reaction pathway analysis**: Density Functional Theory Analysis of reaction pathay of Iodocyclization reaction involving several allylhydroxy precursurs

- **Specialisation & Area of Interests:**

I got my University degree from IIT Kanpur and worked under the supervision Professor S. P. Bhattacharyya, Theory group, Department of Physical Chemistry, IACS, Jadavpur for my Ph.D Thesis. My present Research interest includes:

- Soft computing techniques in molecular electronic structure calculation
- Developing methodology to elucidate the structure, spectral and electronic properties of atomic clusters.
- Development of finite temperature GA based methodology to determine the thermophysical properties
- Application of GA in Molecular modelling

Current Teaching:
Undergraduate Chemistry (specially topics related to Physical Chemistry)

Research Interests:

- Soft computing techniques in molecular electronic structure calculation for the systems with many electrons, Application of Genetic algorithms in the study of docking behaviour of ligand into protein active sites, and the de novo structure design of bioactive molecules.
- Developing methodology to elucidate the structure, spectral and electronic properties of atomic clusters. Specially our interest lies in exploring low lying structures with high curvature and increased strain energy which could lead to solids with unusual intermolecular bonding and electronic properties.

Main Research Projects –

- I was part of DST-NSF project during April-May'2002 and visited the Department of Chemistry, University of Memphis, USA as a Research Fellow at under the exchange programme of DST-NSF project funded by DST, India and NSF, USA
- Completed UGC-MRP project (MRP NO. PSW-115/14-15 Date:02 Feb-2015) during 2015-17 funded by UGC and mobilized a fund of rupees three lakh forty-five thousand

Selected Publications:

- ***Papers***

1. Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm,
2. Pinaki Chaudhuri, Rajendra Saha, S P Bhattacharyya, Chem. Phys. 270, 277 (2001)
3. Direct solution of Schrodinger equation by genetic algorithm:Test cases, Rajendra Saha, Pinaki Chaudhury, S P Bhattacharyya,
4. Phys. Letts. A. 291, 397 (2001)
5. Direct solution of Scrodinger equation by parallel genetic algorthm: Cases of an exactly solvable 2D interacting oscillator
6. Rajendra Saha, S P Bhattacharyya, Christopher Taylor, Young Jhou, T Coundari, Int. J. Quant. Chem. 94, 243 (2003)
7. 4. On solving Schrodinger equation for the ground state of a two-electron atom using genetic algorithm, Rajendra Saha, S
8. Bhattacharyya, Current Science, 86, 960 (2004)
9. 5. On directly solving radial Scrodinger equation for the ground states of two electron atoms or ions by genetic algorithm Rajendra
10. Saha and S P Bhattacharyya, J. Theo. Comp. Chem. 3, 325 (2004)
11. 6. On directly solving Schrodiger equation for H2+ ion by genetic algorithm, Rajendra Saha and S P Bhattacharyya, Int. J. Mod.
12. Phys. C. 18, 163 (2007)
13. 7. Computaition of molecular electronic structure by Genetic Algorithm, Rahul Sharma, Rajendra Saha, Subhajit Nandy, S P
14. Bhattacharyya, Pinaki Chaudhuri, Materials and Manufacturing processes, 24, 155 (2009)
15. 8. Genetic Algorithm based study of Structure and Vibrational spectroscopy of alkali matal ion-water clusters, Rajendra Saha,
16. Aereole: An Academic journal, 2013

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Professional Memberships and Activities:

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