FACULTY MEMBERS' ACADEMIC PROFILE

1. **Name of the Faculty member:** Dr. Soumya Ganguly Neogi
2. **Designation:** Assistant Professor
3. **Qualification:** M.Sc., Ph.D
4. **Specialization:** Physical Chemistry
5. **E-mail address:** soumyagn44@gmail.com
6. **Date of Joining in W.B.E.S.:** **14.12.2015**
7. **Date of Joining in this College:** **15.05.2026**
8. **Previous Colleges Served:** **Chandernagore College**
9. **Total Teaching experience at the college level:** 10 yrs 6 months
10. **Research interests:** Computational Chemistry
11. **Title of thesis (Ph.D.) with year:** **A combined stochastic optimization and quantum chemical method-based study of structure and properties of atomic and molecular clusters (2015)**
10. **Research guidance:** Nil
11. **Research Projects (Completed and ongoing):** Nil
12. **List of publications:**

A) Published papers in Journals:

1. Structure and spectroscopy of water-fluoride microclusters: A combined genetic algorithm and DFT-based study **S. G.Neogi**, P. Chaudhury *J. Comput. Chem* **2012**, 33, 629—639

2.Structure & spectroscopic aspects of water-halide ion clusters:A study based on a conjunction of stochastic & quantum chemical methods **S. G. Neogi**, P Chaudhury *J. Compu. Chem* **2013**, 34, 471-491

3. Structural and spectroscopic studies of carbon dioxide clusters: a combined genetic algorithm and DFT based study **SG Neogi**, S Talukder, P Chaudhury *Structural Chemistry* **2014**, 25, 909—918

4. Structure, spectroscopy and electronic properties of neutral lattice-like $(MgO)_n$ clusters: a study based on a blending of DFT with stochastic algorithms inspired by natural processes *Structural Chemistry* **S. G. Neogi**, P. Chaudhury **2014**, 25, 1229—1244

5.Structural, spectroscopic aspects, and electronic properties of $(TiO_2)_n$ clusters: A study based on the use of natural algorithms in association with quantum chemical methods **S. G.Neogi**, P. Chaudhury *J. Comput. Chem* **2014**, 35, 51—61

6. Structural & spectroscopic studies of water-alkaline earth ion micro clusters: an alternate approach using genetic algorithm in conjunction with quantum chemical methods **S. G. Neogi**, P. Chaudhury *Indian Journal of Physics* **2014,** 88 (8), 781-793

7.Investigation of plausible mechanistic pathways in hydrogenation of η^5-$(C_5H_5)_2Ta(H)=CH_2$: an analysis using DFT & AIM techniques **S. G. Neogi**, A Das, P Chaudhury *J. Mol. Mod.* **2014**, 20, 2132

8.Structure, electronic properties and vibrational spectra of $(MgF_2)_n$ clusters through a combination of genetic algorithm & DFT-based approach **S G Neogi**, P Chaudhury *Mol. Phys.***2015**, 113, 3729-3739

9. Study of structure and spectroscopy of water–hydroxide ion clusters: A combined simulated annealing and DFT-based approach S Guha, **S. G. Neogi**, P Chaudhury *J. Chem Sci.* **2014,** 126, 659-675

10. A parallel tempering-based study of Coulombic explosion and identification of dissociating fragments in charged noble gas clusters S Talukder, S Sen, **S G Neogi**, P Chaudhury *J. Chem. Phys* **2013,** 139, 164312

11. Structure, Carbonyl Vibrational Frequencies, and Local Energy Decomposition of Binding Energy in Formaldehyde Clusters, $(HCHO)_{n=1-10}$ **S G Neogi**, Md. M. Alam *J. Phys. Chem. A* **2022**, 126, 416-423

B) Conference Proceedings: NIL

13. Membership of Learned Societies/ Editorial Boards, etc.:

Indian Chemical Society

Indian society for Radiation and Photochemical Sciences

14. Patents: Nil

15. Awards: Nil

16. Other notable activities: NIL

17. Participation in

A) Seminars/Symposia/Conferences/Workshops:

1. CECAM Flagship school "First steps with SIESTA: from zero to hero" held online from 2nd to 6th October **2023**, Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

2.Seven-day hands on Next-Generation Atomistic Modelling and Simulations with AMS Software workshop organized by Nyro research India Pvt Ltd from **Sept 25th to Oct 4th 2023.**

3. One-day International Seminar on Sedentary Lifestyle, Food Habits and Health Hazards: Challenges of the 21st Century to be held on **8 May 2022** at Chandernagore College, Chandernagore, Hooghly - 712 136, W.B.

4. One-week international workshop on Nano-Materials Modelling using Machine Learning and Siesta (NMM2023) held at Govt. PG College Bilaspur, Himachal Pradesh **14th to 19th April 2023**

5. International Seminar on "Innovation, Expansion, Impacts and Challenges in Chemical and Biological Sciences" (ICBS-2024) Organized by Department of Chemistry, Surendranath College on **22.12.2023**

6. Certificate Program in Density Functional Theory based Studies on Nanomaterials for Optoelectronic

Devices organized by Chhattisgarh Swami Vivekanand Technical University (CSVTU), Bhilai from **03.04.2024 to 13.05.2024**

7. International Seminar on Present Scenario of Chemistry-Biology Interface Research: Issues and Challenges on **19th January, 2024** 10.30 am onwards Organized by Department of Chemistry, Bidhan Chandra College, Asansol, WB, India.

B) OP/RC:

Name of the Course/Summer School	Place	Duration	Sponsor-ing Agency
Faculty Induction Programme FIP-01	GUWAHATI UNI-VERSITY, HRDC	02.09.2020--01.10.2020	UGC
Refresher Programme in Chemistry	IIT DHANBAD	08.06.2018-28.06.2018	MHRD
Refresher Course in Chemistry	Ranchi University	17.08.2021-30.08.2021	UGC