P U L A K N A S K A R

Designation : Assistant Professor
Affiliation : Department of Chemistry, Shyampur Siddheswari Mahavidyalaya,
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Educational Qualification:

Examination	University/Institute	Year	Marks
B.Sc. (Chemistry Hons.)	Derozio Memorial College (under West Bengal State University)	2012	55.75 %
M.Sc. (Specialisation in Physical Chemistry)	Ramakrishna Mission Vivekananda Centenary College (under West Bengal State University)	2014	70.00 %
Ph.D.	University of Calcutta	2019	–
B.Ed.	The West Bengal University of Teachers' Training, Education Planning and Administration (now Baba Saheb Ambedkar Education University)	2023	83.30 %

Research Background:

Type of Research	Supervisor	University/Institute	Topic	Duration
Ph.D.	Prof. Pinaki Chaudhury	Department of Chemistry, University of Calcutta	Quantum-Chemical Studies Of Selected Problems Using Evolutionary Algorithms	16-Oct -2014 To 18-Dec-2019

Current Research Interest(s) : Computational and theoretical chemistry
(Google scholar link : https://scholar.google.co.in/citations?user=WyaLEEoAAAAJ&hl=en)

Other Important Awards/Achievements :

- **Qualified NET** (National Eligibility Test), December 2013 and awarded **CSIR-JRF fellowship** by CSIR-UGC (Govt. of India) (AIR 95)
- **Qualified GATE**, 2022

Symposium / Seminar / Workshop :

- Recent Trends In Macromolecular Chemistry, International Seminar, Activity: Poster Presentation, Date: 10-Jan-2018.
- Current Perspectives in Chemical Research, National Seminar, Activity: Participate, Date: 30-Mar-2016
- Facets Of Chemistry In Biology, National Seminar, Activity: Poster Presentation, Date: 22-Feb-2016 to 23-Feb-2016
- Perspective in Teaching & Research in Physical Chemistry – 2015, National Seminar, Activity: Poster Presentation, Date: 21-Aug-2015 to 22-Aug-2015
- Electronic Structure, Atomistic and Statistical Modelling in Chemistry, Materials and Life Sciences, National Workshop, Activity: Participate, Date: 20-Oct-2014 to 22-Oct-2014
- Modern Trends in Chemistry, State level Seminar, Activity: Participate, Date: 09-Jan-2013

Research Publications :

16. **Energetics and spectroscopic studies of $CNO^{(-)}(H_2O)_n$ clusters and the temperature dependencies of the isomers: An approach based on a combined recipe of parallel tempering and quantum chemical methods**; Pulak Naskar and Srijeeta Talukder*, **J. Comput. Chem.**, 2024, *45*, 2749-2763. DOI: 10.1002/jcc.27480; ISSN: 0192-8651 (Print); 1096-987X (Web). Accepted: 30 July 2024, Published: 16 August 2024.

15. **Dissociation of HF molecule in position and momentum representation by an optimally controlled polychromatic field: study in the dual space using simulated annealing**; Dipayan Seal, Pulak Naskar, Pinaki

Chaudhury and Subhasree Ghosh*, **Mol. Phys.**, 2022, *120*, e2131645. DOI: 10.1080/00268976.2022.2131645; ISSN: 0026-8976 (Print); 1362-3028 (Web). Accepted: 23 September 2022, Published: 13 October 2022.

14. **A two state model study of photo-detachment dynamics driven by an optimally designed polychromatic field: A simulated annealing based optimisation**; Srijeeta Talukder, Dipayan Seal, Pulak Naskar, Pinaki Chaudhury and Subhasree Ghosh*, **Int. J. Quantum Chem.**, 2021, *121*, e26676. DOI: 10.1002/qua.26676; ISSN: 0020-7608 (Print); 1097-461X (Web). Accepted: 30 March 2021, Published: 21 April 2021.

13. **An investigation on the structure, spectroscopy and thermodynamic aspects of $Cl_2^{(-)}(H_2O)_n$ clusters: A combined Parallel tempering and DFT based study**; Sankar Ghorai, Pulak Naskar and Pinaki Chaudhury*, **Int. J. Quantum Chem.**, 2020, *120*, e26270. DOI: 10.1002/qua.26270; ISSN: 0020-7608 (Print); 1097-461X (Web). Accepted: 21 April 2020, Published: 24 June 2020.

12. **Construction of elementary reaction paths of pure and mixed Argon Xenon clusters: A Parallel tempering based study**; Sankar Ghorai*, Pulak Naskar and Pinaki Chaudhury, **Struct. Chem.**, 2020, *31*, 1429-1439. DOI: 10.1007/s11224-019- 01486-8; ISSN: 1040-0400 (Print); 1572-9001 (Web). Accepted: 30 December 2019; Published: 19 February 2020.

11. **Structural transformation in $(MgO)_n$ clusters using a gradient only strategy and its comparison with a full Hessian based calculation**; Rijaul Haque Mirdha, Pulak Naskar and Pinaki Chaudhury*, **Indian J. Phys.**, 2021, *95*, 561-570. DOI: 10.1007/s12648-020-01724-4; ISSN: 0973-1458 (Print); 0974-9845 (Web). Accepted: 25 November 2019, Published: 18 March 2020.

10. **Constructing transformation paths for conformational changes in $(MgF_2)_n$ clusters using a stochastic procedure**; Rijaul Haque Mirdha, Pulak Naskar and Pinaki Chaudhury*, **Mol. Phys.**, 2020, *118*, e1645368. DOI: 10.1080/00268976.2019.1645368; ISSN: 0026-8976 (Print); 1362-3028 (Web). Accepted: 26 June 2019, Published: 28 July 2019.

9. **Controlling the isomerisation dynamics of iodide acetonitrile dimer complex by optimally designed electromagnetic field: a wave packet based approach**; Pulak Naskar, Srijeeta Talukder, Subhasree Ghosh and Pinaki Chaudhury*, **Int. J. Quantum Chem.**, 2019, *119*, e25927. DOI: 10.1002/qua.25927; ISSN: 0020-7608 (Print); 1097-461X (Web). Accepted: 20 February 2019, Published: 13 March 2019. G-Drive: 10.1002qua25927@gmail.com

8. **Structural and spectroscopic aspects of $SCN^{(-)}(H_2O)_n$ clusters and the temperature dependency of the isomers: a parallel tempering based approach**; Pulak Naskar, **Mol. Phys.**, 2019, *117*, 575-589. DOI: 10.1080/00268976.2018.1528395; ISSN: 0026-8976 (Print); 1362-3028 (Web). Accepted: 12 September 2018, Published: 29 September 2018

7. **Role Of Vibrational Contribution In Coulomb Explosion Of Dicationic Neon Gas Clusters : A Parallel Tempering Based Study**; Sankar Ghorai, Pulak Naskar and Pinaki Chaudhury*, **Phys. Chem. Chem. Phys.**, 2018, *20*, 22379-22386. DOI: 10.1039/c8cp03779e; ISSN: 1463-9076 (Print); 1463-9084 (Web). Accepted: 01 August 2018, Published: 13 August 2018.

6. **The effect of stochastic barrier fluctuation on semiclassical transmission probability and Shannon entropy of a symmetric double well potential**; Pulak Naskar, Srijeeta Talukder, Pinaki Chaudhury and Subhasree Ghosh*, **Int. J. Quantum Chem.**, 2018, *118*, e25667. DOI: 10.1002/qua.25667; ISSN: 0020-7608 (Print); 1097- 461X (Web). Accepted: 20 April 2018, Published: 13 August 2018.

5. **Structural, spectroscopic and thermodynamic aspects of azide-water clusters: an approach using a conjugated prescription of stochastic and quantum chemical methods**; Pulak Naskar*, Rituparna Roy, Srijeeta Talukder and Pinaki Chaudhury*, **Mol. Phys.**, 2018, *116*, 2172-2186. DOI: 10.1080/00268976.2018.1465605; ISSN: 0026-8976 (Print); 1362-3028 (Web). Accepted: 05 April 2018, Published: 09 May 2018.

4. **Mapping out reaction paths for conformational changes in $(MgO)_n$ clusters: a study based on a stochastic procedure**; Rijaul Haque Mirdha, Pulak Naskar, and Pinaki Chaudhury*, **Struct. Chem.**, 2018, *29*, 523-532. DOI: 10.1007/s11224-017-1049-1; ISSN: 1040-0400 (Print); 1572-9001 (Web). Accepted: 22 October 2017, Published: 02 November 2017.

3. **An adaptive mutation simulated annealing based investigation of Coulombic explosion and identification of dissociation patterns in $(CO_2)_n^{2+}$ clusters**; Pulak Naskar, Srijeeta Talukder* and Pinaki Chaudhury*, **Phys. Chem. Chem. Phys.**, 2017, *19*, 9654-9668. DOI: 10.1039/c7cp00655a; ISSN: 1463-9076 (Print); 1463-9084 (Web). Accepted: 14 March 2017, Published: 15 March 2017.

2. **An investigation on the structure, spectroscopy and thermodynamic aspects of $Br_2^{(-)}(H_2O)_n$ clusters using a conjunction of stochastic and quantum chemical methods**; Pulak Naskar and Pinaki Chaudhury*, Phys. Chem. Chem. Phys., 2016, *18*, 16245-16257. DOI: 10.1039/c6cp01960a; ISSN: 1463-9076 (Print); 1463-9084 (Web). Accepted: 17 May 2016, Published: 18 May 2016.

1. **Structural and spectroscopic studies of iodine dimer radical anion hydrated clusters: an approach using a combination of stochastic and quantum chemical methods**; Pulak Naskar* and Pinaki Chaudhury*, **RSC Adv.**, 2016, *6*, 12315-12325. DOI: 10.1039/c5ra19763e; ISSN: 2046-2069. Accepted: 12 January 2016, Published: 18 January 2016.

09-Jan-2025
Pulak Naskar