Dr. Tapas Sahoo

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Profile Summary

A dedicated researcher and educator with expertise in quantum molecular dynamics, computational chemistry, and high-performance computing simulations. Skilled in developing innovative algorithms and mathematical models to tackle complex chemical systems. Passionate about teaching and fostering scientific curiosity in students.

Present Position

Designation **Temporary Faculty**
Department of Chemistry,
National Institute of Technology (NIT) Raipur,
G.E. Road, Raipur - 492010 (C.G.), India.

Personal

Born **January 15, 1984**
Gender **Male**
Citizen **Indian**

Education

2002–2006 **B.Sc. (honors) in Chemistry**
Ramakrishna Mission Vivekananda Centenary College, Rahara,
University of Calcutta.
Percentage: *68.375%*

2006–2008 **M.Sc. in Chemistry**,
Specialization: Physical Chemistry
Rajabazar Science College,
University of Calcutta.
Percentage: *69.8%*

June 22, 2008 **Joint CSIR-UGC Test for Junior Research Fellowship**, *and*
Eligibility for Lectureship (NET) in Chemical Sciences
under **CSIR Fellowship** scheme.

2008–2015 **Ph.D. in Chemistry (Physical)**
Indian Association for the Cultivation of Science, Kolkata, India.

Ph.D. Thesis

Title	"Surface temperature effect on the molecule-surface scattering processes and the reactive scattering for triatomic system"
Supervisor	Professor Satrajit Adhikari
Degree received on	January 7, 2015 from the University of Calcutta.

Research Experience

May 10, 2022–December 31, 2023 — **Post Doctoral Research Associate-III**, *S. N. Bose National Centre for Basic Sciences*, Kolkata, India.
Quantum molecular dynamics simulations for complex molecular systems.

November 1, 2016 – August 31, 2021 — **Postdoctoral Fellow**, *Department of Chemistry*, University of Waterloo, Canada.
Quantum molecular dynamics simulations for complex molecular systems;
Mathematical modeling;
Parallel algorithmic developments;
Computations of ground-state energetic, structural properties;
Estimations of entanglement entropy.

July 6, 2014 – July 6, 2016 — **Postdoctoral Fellow**, *Department of Chemical and Biological Physics*, Weizmann Institute of Science, Israel.
Theoretical formulation of atom-surface scattering process;
Classical perturbation theory for energy-loss distribution;
Classical trajectory calculation.

Fellowships

- **DST-SERB International Travel Grant Award** in 2011.
- Dean's support of **postdoctoral fellowship**, Weizmann Institute of Science from 2014-2016.
- **Postdoctoral fellowship**, University of Waterloo, Canada from November, 2016 to August, 2021.
- **Postdoctoral fellowship**, S. N. Bose National Centre for Basic Sciences, Kolkata, India from May, 2022 to till date.

Research Interests

- Quantum molecular dynamics of many–body systems, mathematical modelling, algorithmic developments and high performance computing simulations of complex molecular systems.
- Computation of entanglement entropy for confined molecular systems.
- Estimation of thermodynamic as well as ground state properties of many–body systems by employing Path Integral Monte Carlo methodology.
- Effect of nuclear spin in many-body rotors.
- Molecular dynamics for material science.

Teaching Experience

National Institute of Technology (NIT) Raipur, (February 5, 2024 – Present)
Temporary Faculty, Department of Chemistry

- **Taught PG courses (Two (2) semesters)**: Thermodynamics, Electrochemistry, Quantum Mechanics, and Chemical Kinetics.
- **Delivered B.Tech. lectures (Two (2) semesters)**: Applied Chemistry (one semester), Environment and Ecology (one semester).
- Supervised B.Tech. laboratory sessions.
- Developed course materials, assessments, and provided constructive feedback.

Key Skills

Programming languages	FORTRAN, Python, C, C++, julia ...
	Object-Oriented Programming in C++ and Python
Web Development	HTML, CSS, JavaScript
Program building tool	Makefile
Scripting languages	Python, Bash ...
High-performance computations	OpenMP, MPI
Version Control	Git, Github
Research Tools	Gnuplot, Matplotlib, netCDF, Matlab, Mathematica,
	Visual Molecular Dynamics, MoRiBS-PIGS,
	PySCF, ORCA, MCTDH.
Scientific Writing tools	LaTeX, LyX, pgf/TikZ.

Publications

Preprints (Not Peer Reviewed)

* indicates equal contributions
† indicates corresponding author(s) (if not the senior author)
boldface indicates a member of my lab

[1] **Tapas Sahoo**†, "Comparison of physical processes of atom-surface scattering computed by classical and quantum dynamics", arXiv: 2306.17483 (quant-ph), 2023.

Journal Articles (Peer Reviewed)

* indicates equal contributions
† indicates corresponding author(s) (if not the senior author)
boldface indicates a member of my lab

[2] **Tapas Sahoo**†, "A Path Integral Monte Carlo Approach for Confined Rigid Linear Rotors with Nuclear Spin Symmetry: Application to Hydrogen Chains", *Molecular Physics*(), Year 2025. Manuscript under review.

[3] **Tapas Sahoo**† and Gautam Gangopadhyay, "Effect of neighbouring molecules on ground-state properties of many-body polar linear rotor systems", *Molecular Physics*, Taylor & Francis, Vol. 121 (24), Year 2023, pp. e2242967, DOI 10.1080/00268976.2023.2242967. (Impact Factor: 1.6, Quartile Ranking: Q3).

[4] Sandip Ghosh, **Tapas Sahoo**, Michael Baer, and Satrajit Adhikari, "Charge transfer processes for $H + H_2^+$ reaction employing coupled 3D wavepacket approach on beyond Born–Oppenheimer based *ab initio* constructed diabatic potential energy surfaces", *The Journal of Physical Chemistry A*, ACS Publications, Vol. 125 (3), Year 2021, pp. 731–745, DOI https://doi.org/10.1021/acs.jpca.0c08975. (Impact Factor: 2.7, Quartile Ranking: Q2).

[5] **Tapas Sahoo**, Tobias Serwatka, and Pierre-Nicholas Roy, "A path integral ground state approach for asymmetric top rotors with nuclear spin symmetry: Application to water chains", *The Journal of Chemical Physics*, AIP Publishing LLC, Vol. 154 (24), Year 2021, pp. 244305, DOI https://doi.org/10.1063/5.0053051. (Impact Factor: 3.1, Quartile Ranking: Q1).

[6] **Tapas Sahoo**, Dmitri Iouchtchenko, CM Herdman, and Pierre-Nicholas Roy, "A path integral ground state replica trick approach for the computation of entanglement entropy of dipolar linear rotors", *The Journal of Chemical Physics*, AIP Publishing LLC, Vol. 152 (18), Year 2020, pp. 184113, DOI https://doi.org/10.1063/5.0004602. (Impact Factor: 3.1, Quartile Ranking: Q1).

[7] Bijit Mukherjee, Koushik Naskar, Soumya Mukherjee, Sandip Ghosh, **Tapas Sahoo**, and Satrajit Adhikari, "Beyond Born–Oppenheimer theory for spectroscopic and scattering processes", *International Reviews in Physical Chemistry*, Taylor & Francis, Vol. 38 (3-4), Year 2019, pp. 287–341, DOI https://doi.org/10.1080/0144235X.2019.1672987. (Impact Factor: 2.5, Quartile Ranking: Q2).

[8] Sandip Ghosh, **Tapas Sahoo**, Satrajit Adhikari, Rahul Sharma, and António J C Varandas, "Coupled 3D time-dependent wave-packet approach in hyperspherical coordinates: The $D^+ + H_2$ reaction on the triple-sheeted DMBE potential energy surface", *The Journal of Physical Chemistry A*, ACS Publications, Vol. 119 (50), Year 2015, pp. 12392–12403, DOI https://doi.org/10.1021/acs.jpca.5b07718. (Impact Factor: 2.7, Quartile Ranking: Q2).

[9] Souvik Mandal, **Tapas Sahoo**, Sandip Ghosh, and Satrajit Adhikari, "The effect of phonon modes and electron–hole pair couplings on molecule–surface scattering processes", *Journal of Theoretical and Computational Chemistry*, World Scientific, Vol. 14 (04), Year 2015, pp. 1550028, DOI https://doi.org/10.1142/S0219633615500285. (Impact Factor: 2.0, Quartile Ranking: Q3).

[10] Souvik Mandal, **Tapas Sahoo**, Sandip Ghosh, and Satrajit Adhikari, "The effect of surface temperature for the scattering of D_2(v=0, j=0)-Cu(111) system: A spherical polar TDDVR approach", *Journal of the Indian Chemical Society*, Scientific Publishers, Vol. 92 (3), Year 2015, pp. 291–303. (Impact Factor: 3.2, Quartile Ranking: Q4).

[11] Souvik Mandal, **Tapas Sahoo**, Sandip Ghosh, and Satrajit Adhikari, "The effect of surface temperature on H_2/D_2(v=0, j=0)-Ni(100) scattering processes", *Molecular Physics*, Taylor & Francis, Vol. 113 (19-20), Year 2015, pp. 3042–3056, DOI https://doi.org/10.1080/00268976.2015.1074741. (Impact Factor: 1.6, Quartile Ranking: Q3).

[12] **Tapas Sahoo**, Sandip Ghosh, Satrajit Adhikari, Rahul Sharma, and António J C Varandas, "Low-temperature $D^+ + H_2$ reaction: A time-dependent coupled wave-packet study in hyperspherical coordinates", *The Journal of Chemical Physics*, AIP Publishing LLC, Vol. 142 (2), Year 2015, pp. 024304, DOI https://doi.org/10.1063/1.4905379. (Impact Factor: 3.1, Quartile Ranking: Q1).

[13] **Tapas Sahoo** and Eli Pollak, "Second order classical perturbation theory for the sticking probability of heavy atoms scattered on surfaces", *The Journal of Chemical Physics*, AIP Publishing LLC, Vol. 143 (6), Year 2015, pp. 064706, DOI https://doi.org/10.1063/1.4928432. (Impact Factor: 3.1, Quartile Ranking: Q1).

[14] **Tapas Sahoo**, Sandip Ghosh, Satrajit Adhikari, Rahul Sharma, and Antönio J C Varandas, "Coupled 3D time-dependent wave-packet approach in hyperspherical coordinates: Application to the adiabatic singlet-State ($1^1A'$) $D^+ + H_2$ reaction", *The Journal of Physical Chemistry A*, ACS Publications, Vol. 118 (26), Year 2014, pp. 4837–4850, DOI https://doi.org/10.1021/jp5035739. (Impact Factor: 2.7, Quartile Ranking: Q2).

[15] **Tapas Sahoo**, Sandip Ghosh, Satrajit Adhikari, Rahul Sharma, and Antönio J.C. Varandas, "Erratum: Coupled 3D time-dependent wave-packet approach in hyperspherical coordinates: Application to the adiabatic singlet-State ($1^1A'$) $D^+ + H_2$ reaction (Journal of Physical Chemistry A 118, 26 (4837-4850))", *Journal of Physical Chemistry A*, American Chemical Society, Vol. 118 (33), Year 2014, pp. 6740, DOI 10.1021/jp506654u. (Impact Factor: 2.7, Quartile Ranking: Q2).

[16] Basir Ahamed Khan, Subhankar Sardar, **Tapas Sahoo**, Pranab Sarkar, and Satrajit Adhikari, "Nearly linear scalability of time-dependent discrete variable representation (TD-DVR) method for the dynamics of multi-surface multi-mode hamiltonian", *Journal of Theoretical and Computational Chemistry*, World Scientific, Vol. 12 (05), Year 2013, pp. 1350042, DOI https://doi.org/10.1142/S0219633613500429. (Impact Factor: 2.0, Quartile Ranking: Q3).

[17] Bhavesh K Shandilya, Shrabani Sen, **Tapas Sahoo**, Srijeeta Talukder, Pinaki Chaudhury, and Satrajit Adhikari, "Selective bond breaking mediated by state specific vibrational excitation in model HOD molecule through optimized femtosecond IR pulse: A simulated annealing based approach", *The Journal of Chemical Physics*, American Institute of Physics, Vol. 139 (3), Year 2013, pp. 034310, DOI https://doi.org/10.1063/1.4813127. (Impact Factor: 3.1, Quartile Ranking: Q1).

[18] Anita Das, **Tapas Sahoo**, Debasis Mukhopadhyay, Satrajit Adhikari, and Michael Baer, "Dressed adiabatic and diabatic potentials to study conical intersections for F + H_2", *The Journal of Chemical Physics*, American Institute of Physics, Vol. 136 (5), Year 2012, pp. 054104, DOI https://doi.org/10.1063/1.3679406. (Impact Factor: 3.1, Quartile Ranking: Q1).

[19] **Tapas Sahoo**, Saikat Mukherjee, and Satrajit Adhikari, "Surface temperature effect on the scattering of D_2(v=0, j=0)-Cu(111) system", *The Journal of Chemical Physics*, American Institute of Physics, Vol. 136 (8), Year 2012, pp. 084306, DOI https://doi.org/10.1063/1.3687175. (Impact Factor: 3.1, Quartile Ranking: Q1).

[20] **Tapas Sahoo**, Subhankar Sardar, and Satrajit Adhikari, "The effect of phonon modes on the D_2(v=0, j=0)-Cu(111) scattering processes", *Physica Scripta*, IOP Publishing, Vol. 84 (2), Year 2011, pp. 028105, DOI doi:10.1088/0031-8949/84/02/028105. (Impact Factor: 2.6, Quartile Ranking: Q2).

[21] **Tapas Sahoo**, Subhankar Sardar, and Satrajit Adhikari, "The effect of phonon modes on the H_2(v, j)/D_2(v, j)-Cu(1nn) scattering processes", *Physical Chemistry Chemical Physics*, Royal Society of Chemistry, Vol. 13 (21), Year 2011, pp. 10100–10110, DOI https://doi.org/10.1039/C0CP00336K. (Impact Factor: 2.9, Quartile Ranking: Q1).

[22] **Tapas Sahoo**, Subhankar Sardar, Padmabati Mondal, Biplab Sarkar, and Satrajit Adhikari, "Effect of surface modes on the six-dimensional molecule-surface scattering dynamics of H_2-Cu(100) and D_2-Cu(111) systems", *The Journal of Physical Chemistry A*, ACS Publications, Vol. 115 (21), Year 2011, pp. 5256–5273, DOI https://doi.org/10.1021/jp201524x. (Impact Factor: 2.7, Quartile Ranking: Q2).

Conference Presentations

Oral Presentations

- Computation of entanglement entropy for rotors. Delivered an **invited lecture** in *Quantum Sensing & Quantum Metrology (QSQM-2023)* jointly organized by Indian Association for the Cultivation of Science, Kolkata and Indian Institute of Science Education and Research, Kolkata held on December 4-6, 2023.
- A path integral ground state approach for asymmetric top rotors with nuclear spin symmetry. Delivered an **invited lecture** at the *Theoretical Chemistry Meeting: Structure and Dynamics* organized by Indian Association for the Cultivation of Science, Kolkata, India, during May 26-29, 2022.
- Estimation of ground state entanglement entropy for continuous rotational degrees of freedom: A Path Integral Replica Trick approach. Delivered an **invited lecture** at the *Shanghai New York University, Shanghai, China* on June 11, 2019.
- Estimation of ground state entanglement entropy for continuous rotational degrees of freedom: A Path Integral Replica Trick approach. Delivered an **invited lecture** at the *Theoretical Chemistry Symposium 2019* organized by BITS Pilani, India during February 13-16, 2019.
- Estimation of ground state entanglement entropy for continuous rotational degrees of freedom: A Path Integral Replica Trick approach. Delivered an **invited lecture** at the *International Conference of Complex and Functional Materials 2018* organized by SNBNCBS held in Kolkata, West Bengal, India during December 13-16, 2018.

- Second order classical perturbation theory for the sticking probability of heavy atoms scattered on surfaces, **Tapas Sahoo** and Eli Pollak. Talk given at the *Chemical Physics Retreat* organized by Department of Chemical Physics, Weizmann Institute of Science, Israel during March 1-3, 2016.

Poster Presentations

- The 35th Symposium on Chemical Physics at the University of Waterloo: In the honour of Robert J. Le Roy held at Waterloo, ON, Canada during November 1-3, 2019.
- DAE BRNS symposium on Current Trends in Theoretical Chemistry held at Bhabha Atomic Research Centre, Mumbai, India during September 26-28, 2013.
- Structure and Dynamics: Born-Oppenheimer Theories and Applications, Reactions Dynamics and Molecule-surface Scattering held at Indian Association for the Cultivation of Science, Kolkata, India during February 17-20, 2013.
- 9th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2012 held at Bangaluru, India during February 17-19, 2012.
- Diamond Jubilee Symposium on Recent Trends in Chemistry held at IIT Kharagpur, West Bengal, India during October 21-22, 2011.
- **2011 Gordon Research Conferences: Dynamics at Surfaces** held at Salve Regina University in Newport, Rhode Island, USA during August 7-12, 2011.
- 8th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2011 held at Corbett Hideaway, Jim Corbett National Park, Uttarakhand, India during February 18-20, 2011.
- Computational Techniques in Soft Matter 2010 (CTSM10) held at S N Bose National Centre For Basic Sciences, Kolkata, India from December 6-10, 2010.
- 7th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2010 held at International Centre Goa, Dona Paola, Goa, India from February 18-21, 2010.
- RAMET-2010 held at Sankarpur, West Bengal, India during January 5-8, 2010.
- 6th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2009 held at Mandarmoni, West Bengal, India during February 20-22, 2009.

References

- **Dr. Satrajit Adhikari**, Senior Professor
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- **Dr. Deb Shankar Ray**, Senior Professor
  School of Chemical Sciences
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