

# Dr. Tapas Sahoo

Temporary Faculty at NIT Raipur

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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	<b>Post Doctoral Research Associate-III, S. N. Bose National Centre for Basic Sciences, Kolkata, India.</b> Quantum molecular dynamics simulations for complex molecular systems.
November 1, 2016 – August 31, 2021	<b>Postdoctoral Fellow, Department of Chemistry, University of Waterloo, Canada.</b> 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	<b>Postdoctoral Fellow, Department of Chemical and Biological Physics, Weizmann Institute of Science, Israel.</b> 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.

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## Key Skills

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

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## 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**<sup>†</sup>, “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**<sup>†</sup>, “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**<sup>†</sup> 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<sub>2</sub><sup>+</sup> 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<sup>+</sup> + H<sub>2</sub> 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<sub>2</sub>(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<sub>2</sub>/D<sub>2</sub>(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<sup>+</sup> + H<sub>2</sub> 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 António J C Varandas, "Coupled 3D time-dependent wave-packet approach in hyperspherical coordinates: Application to the adiabatic singlet-State (1<sup>1</sup>A') D<sup>+</sup> + H<sub>2</sub> 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 António J.C. Varandas, "Erratum: Coupled 3D time-dependent wave-packet approach in hyperspherical coordinates: Application to the adiabatic singlet-State (1<sup>1</sup>A') D<sup>+</sup> + H<sub>2</sub> 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](https://doi.org/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<sub>2</sub>", *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<sub>2</sub>(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<sub>2</sub>(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<sub>2</sub>(v, j)/D<sub>2</sub>(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, Biplob Sarkar, and Satrajit Adhikari, "Effect of surface modes on the six-dimensional molecule-surface scattering dynamics of H<sub>2</sub>-Cu(100) and D<sub>2</sub>-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 Bangalore, 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.

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#### References

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