Subhasish Mallick

CONTACT INFORMATION

Vill: Aramdanga, P.O.: Asharu, P.S.: Bongaon
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West Bengal,

India, 743251
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NATIONALITY **Indian**

DATE OF BIRTH **29-12-1992**

RESEARCH INTERESTS **Electronic Structure, Density Functional Theory (DFT), Reaction Kinetics and Dynamics, $Ab-initio$ Molecular Dynamics, Classical Molecular Dynamics for Biophysical Systems, Reaction on Water Surface, Tunneling, Quantum Confinement.**
Google Scholar
Scopus ID

EDUCATION

Ph.D., Theoretical and Computational Chemistry (July 2016 to October 2021)
Malaviya National Institute of Technology Jaipur, Rajasthan, India

- **Dissertation Topic: "Theoretical Understanding of $OH^{\bullet}$+ HCl Reaction: Atmospheric Impact and Dynamical Implications"**
- **Supervisor: Dr. Pradeep Kumar**

M.Sc., Chemistry, 2013-2015
Sree Chaitanya College Habra, West Bengal, India

B.Sc., Chemistry (Hons.) 2010-2013
Bhairab Ganguly College, West Bengal, India

HONORS AND AWARDS **Qualified GATE, CSIR-UGC NET.**

ACADEMIC EXPERIENCE

Postdoc Fellow, August 2021 to Present
The Hebrew University of Jerusalem, Jerusalem, Israel

- **Supervisor: Prof. Noam Agmon**

PUBLICATIONS

26. Mallick, S. Ion-Lipid interactions in biomembranes (*Manuscript submitted*).

25. Mallick, S and Agmon, N. Multi-Proton dynamics near membrane-water interface. *Nat. Commun.*, 2025 16 (1), 3276 (*Featured among the Editors' Highlights: Best 50 Articles in Nat. Commun. Click here for link*).

24. Ali M. S., Ali M. S., Mallick, S, Bhandari S., Roy B., Karmakar S., Chattopadhyay S., Chattopadhyay D. Dual Parameter Smart Sensor for Nitrogen and Temperature Sensing Based on Defect-Engineered 1T-MoS_2. *Sci. Rep.*, 2024 14 (1), 21469.

23. Mallick, S and Agmon, N. Lateral diffusion of ions near membrane. *Phys. Chem. Chem. Phys.*, 2024 26, 19433–19449.

22. Yadav, P., Rai, P. K.,Mallick, S and Kumar, P. External electric field to control the Diels–Alder reactions of endohedral fullerene. *Phys. Chem. Chem. Phys.*, 2022 18(24), 11131-11136.

21. Kumar, A,Mallick, S and Kumar, P. Nitrous acid (HONO) as a sink of the simplest Criegee intermediate in the atmosphere. *Phys. Chem. Chem. Phys.*, 2022 12(24), 7458-7465

20. Mallick, S and Kumar, P. The Effect of Microsolvation on the Mode Selectivity of the $OH^\bullet$ + HCl Reaction. *Phys. Chem. Chem. Phys.*, 2021 23(44), 25246-25255

19. Mallick, S, Kumar, A and Kumar, P. Oxidation of $HOSO^\bullet$ by $Cl^\bullet$: a new source of SO_2 in the atmosphere? *Phys. Chem. Chem. Phys.*, 2021 23(34), 18707-18711.

18. Mallick, S, Rai, P. K. and Kumar, P. Accurate Estimation of Singlet-Triplet Gap of Strongly Correlated Systems using CCSD(T) method by Improving the Reference Orbitals, *Comput. Theor. Chem.*, 2021, 113326.

17. Mallick, S, Mishra, B. K., Kumar, P. and Sathyamurthy, N. Effect of Confinement on the Ammonia Inversion. *Eur. Phys. J. D* , 2021, 75(3), 1-10.

16. Mallick, S, Kumar, A and Kumar, P. Oxidation of $HOSO^\bullet$ by $NH_2^\bullet$: A new path for the formation of an acid rain precursor. *Chem. Phys. Lett.*, 2021 , 138536.

15. Mallick, S and Kumar, P. $OH^\bullet$ + HCl Reaction at the Surface of a Water Droplet: An Ab Initio Molecular Dynamical Study. *J Phys. Chem. B*, 2020, 124(12), 2465-2472.

14. Mallick, S and Kumar, P. The reaction of N_2O with the Criegee intermediate: A theoretical study. *Comput. Theor. Chem.*, 2020, 11303.

13. Kumar, A, Mallick, S and Kumar, P. Effect of water on the oxidation of CO by a Criegee intermediate. *Phys. Chem. Chem. Phys.*, 2020 22(37), 21257-21266.

12. Mallick, S, Roy, B and Kumar, P. A comparison of DLPNO-CCSD(T) and CCSD(T) method for the determination of the energetics of hydrogen atom transfer reactions. *Comput. Theor. Chem.*, 2020, 112934.

11. Mallick, S and Kumar, P. Computational evidence for sulfur atom tunneling in the ring flipping reaction of S_4N_4. *Chem. Phys. Lett.*, 2020 , 137440.

10. Mallick, S, Kumar, A and Kumar, P. Kinetic Instability of the Sulfurous Acid in the Presence of Ammonia and Formic Acid. *Phys. Chem. Chem. Phys.*, 2020 , 18646-18654.

9. Kumar, A, Mallick, S, Mishra, B. K. and Kumar, P. Effect of ammonia and formic acid on the $CH_3O^{\bullet} + O_2 \longrightarrow CH_2O + HO_2^{\bullet}$ reaction: A quantum chemical investigation. *Phys. Chem. Chem. Phys.*, 2020 22, 2405-2413.

8. Mallick, S and Kumar, P. Switching of the reaction enthalpy from exothermic to endothermic for decomposition of H_2CO_3 under confinement. *Phys. Chem. Chem. Phys.*, 2019 21(37), 20849-20856.

7. Mallick, S, Kumar, A, Mishra, B. K. and Kumar, P. Influence of water on $CH_3O^{\bullet} + O_2 \longrightarrow CH_2O + HO_2^{\bullet}$ reaction. *Phys. Chem. Chem. Phys.*, 2019 21, 17534.

6. Mallick, S, Kumar, A and Kumar, P. Revisiting the reaction energetics of $CH_3O^{\bullet} + O_2$ ($^3\Sigma^-$) reaction: Crucial role of post-CCSD(T) corrections. *Phys. Chem. Chem. Phys.*, 2019 21, 6559-6565.

5. Mallick, S and Kumar, P. Impact of Post-CCSD(T) Corrections on Reaction Energetics and Rate Constants of the $OH^{\bullet}$ + HCl Reaction. *J Phys. Chem. A*, 2018 122(36), 7151-7159.

4. Mallick, S., Sarkar, S., Bandyopadhyay, B., and Kumar, P. Effect of ammonia-water complex on decomposition of carbonic acid in troposphere: A quantum chemical investigation .*Comput. Theor. Chem.*, 2018 1132, 50-58.

3. Sarkar, S.,Mallick, S., Kumar, P. and Bandyopadhyay, B. Ammonolysis of ketene as a potential source of acetamide in troposphere: A quantum chemical investigation *Phys. Chem. Chem. Phys.*, 2018 19(40), 27848-27858.

2. Sarkar, S.,Mallick, S., Deepak, Kumar, P. and Bandyopadhyay, B. Isomerization of methoxy radical in the troposphere: competition between acidic, neutral and basic catalysts *Phys. Chem. Chem. Phys.*, 2017 19(40), 27848-27858.

1. Mallick, S., Sarkar, S., Bandyopadhyay, B., and Kumar, P. Effect of Ammonia and Formic Acid on the $OH^{\bullet}$+ HCl Reaction in the Troposphere: Competition between Single and Double Hydrogen Atom Transfer Pathways.*J Phys. Chem. A*, 2017 122(1), 350-363.

Conference Presentations and Workshops

- Effect of Ammonia and Formic Acid on the $OH^{\bullet}$+ HCl Reaction in the Troposphere. (Poster) 2^{nd} meeting on Spectroscopy, Structure and Dynamics, held on March, 2018.

- Impact of Post-CCSD(T) Corrections on Reaction Energetics and Rate Constants of the $OH^{\bullet}$ + HCl Reaction. (Poster) 16^{th} edition of Theoretical Chemistry Symposium, held on February, 2019.

- **Switching of the reaction enthalpy from exothermic to endothermic for decomposition of H_2CO_3 under confinement.. (Poster) 16^{th} edition of Spectroscopy and Dynamics of Molecules and Clusters, held on March, 2019.**

- **The reaction energetics of $CH_3O^{\bullet}$ + O_2 ($^3\Sigma^-$) reaction: Crucial role of post-CCSD(T) corrections. (Oral) 3^{rd} meeting on Spectroscopy, Structure and Dynamics, held on April, 2019.**

- **"Fundamentals of C Programming Skills" workshop held on August, 2019.**

- **$OH^{\bullet}$ + HCl Reaction at the Surface of a Water Droplet. (Poster) 17^{th} edition of Spectroscopy and Dynamics of Molecules and Clusters, held on February, 2020.**

- **Interaction and dynamics of ions at membrane surface . (Invited Speaker) "Recent Advances in Chemistry: Theoretical and Computational Aspects" during November 18-20, 2022.**

- **Participated in CECAM flagship school for path integral quantum mechanics during June 4-8, 2023.**

Computer and Software Skills

- **Languages: Fortran, Tcl.**
- **Electronic Structure packages: Gaussian, GAMESS-US, MRCC, ORCA, CFOUR, Quantum Espresso, DFTB+.**
- **Kinetic Calculation Packages: Polyrate, TheRate, Kisthelp, Multiwell, MESMER.**
- **Dynamical simulation code: CP2K, Venus, Gromacs, NAMD.**
- **Visualization Packages: VMD, GaussView, Chemcraft, Mercury, etc.**
- **Operating Systems: Good experience with the most flavors of Linux, Ubuntu, CentOS, Suse. Experienced with HP cluster, Windows.**

Language skills

My mother tongue is Bengali, but almost everything I write is in English for scientific work.
Bengali: Native tongue.
English and Hindi: Fluent.

References

- **Prof. Narayanasami Sathyamurthy**
  Indian Institute of Science Education and Research Mohali
  SAS Nagar 140306, India
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- **Dr. Pradeep Kumar**
  Department of Chemistry
  Malaviya National Institute of Technology Jaipur
  J.L.N Marg, Malviyanagar, Rajasthan, India, 302017
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- **Prof. Noam Agmon**
  Aronberg 126, Givat Ram Campus
  Institute of Chemistry
  The Fritz Haber Research Center for Molecular Dynamics
  The Hebrew University of Jerusalem, Jerusalem, Israel, 9190401
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- **Prof. Ashwani Kumar Tiwari (FRSC)**
  Reaction Dynamics Lab,
  AAC Building, Room No. 302 F,
  Indian Institute of Science Education and Research Kolkata,
  Mohanpur, 741246
  West Bengal, India.
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