Dr. Ambar Banerjee

Curriculum vitae

Personal Details

Date of birth: 27th Nov, 1985 Email: ambarpchem@gmail.com

Permanent Address: 72 J.K. Street, Uttarpara, Hooghly, West Bengal, India.

Present Address: S:t Johannesgatan 26, LGH : 1002, 75312 Uppsala, Sweden.

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Experience

- **Postdoctoral fellow at Uppsala University. (2021-present)**
- **Postdoctoral fellow at Stockholm University. (2019-2021)**
- **Postdoctoral fellow at the Weizmann Institute of Science, Israel. (2018-2019)**
- **Postdoctoral fellow at IACS, Kolkata. (Six Months, Sep/2017-March/2018)**

Publications

Uppsala University

1. Tracking C-H activation with orbital resolution, Jay, R.M., *† **Banerjee, A.,***† Leitner, T., Wang, R., Harich, J., Stefanuik, R., Wikmark, H., Coates, M. R., Beale, E. V., Kabanova, V., Kahraman, A., Wach, A., Ozerov, D., Arrell, C., Johnson, P.J.M., Borca, C.N., Cirelli, C., Bacellar, C., Milne, C., Huse, N., Smolentsev, G., Huthwelker, T,. Odelius, M. & Wernet, P.,*) **[† as equal 1st author] [* as corresponding author]** *Science*, 380, **2023**, *955–960*

2. Triplet Harvesting in Single-bond Connected Donor-acceptor Dyad: A Universal Mechanism. Karak, P., Moitra, T., **Banerjee, A.,*** Ruud, K.,* Chakrabarti, S.,* **2023**, **[* as corresponding author]** ChemRxiv, doi: 10.26434/chemrxiv-2023-z34m0

Stockholm University

3. Photoinduced bond oscillations in ironpentacarbonyl $Fe(CO)_5$ give delayed, synchronous bursts of carbonmonoxide (CO) release, **Banerjee, A.,*** Coates M. R., Kowalewski, M., Wikmark, H., Jay, R. M., Wernet, P., & Odelius, M. *Nature Communications*, *13*(1), **2022**, *1-10.* [* as corresponding author]

4. Simulating fluorine K-edge resonant inelastic X-ray scattering of sulfur hexafluoride and the effect of dissociative dynamics, **Banerjee, A.,** da Cruz, V.V., Ekholm, V., Såthe, C., Rubensson, J.E., Ignatova, N., Gel'mukhanov, F. and Odelius, M., **2023**. ChemRxiv, doi: 10.26434/chemrxiv-2023-865lt (accepted in PRA)

5. Spectroscopic signature of dynamical instability of the aqueous complex in the brown-ring nitrate test. **Banerjee, A.,*** Coates, M. R., & Odelius, M. [* as corresponding author], *Chemistry -A European Journal*, 28, **2022**, *e202200923*

6. The Role of Copper Salts and O_2 in the Mechanism of CΞN Bond Activation for Facilitating Nitrogen Transfer Reactions, Ghosh, B., **Banerjee, A.**, Roy, L., Nath, R., Mann, R. & Paul, A., *Angew. Chem. Int. Ed. 61*, **2022**, e202116868

7. Electronic Structure Changes of an Aromatic Amine Photoacid along the Förster Cycle, Eckert, S., Winghart, M. O., Kleine, C., **Banerjee, A**., Ekimova, M., Ludwig, J., Harich, J., Mitzner, R., Pines, E., Huse, N., Wernet, P., Odelius, M., and T. J. Nibbering E., *Angew. Chem. Int. Ed. , 61*, **2022**, e202200709. (selected Inside Cover)

8. Carbon K edge X-ray Emission Spectroscopy of Gas Phase Ethylenic Molecules. Ingle, R., **Banerjee, A.,** Bacellar, C., Barillot, T., Longetti, L., Coreno, M., de Simone, M., Zuccaro, F., Poletto, L., Miotti, P., Röder, A., Stolow, A., Schuurman, M., Odelius, M., Chergui, M. , *J. Phys. B: At. Mol. Opt. Phys. 55,* **2022**, *044001.*

9. Wave packet theory for non-resonant x-ray emission and non-resonant Auger electron emission in molecules. Savchenko, V., Odelius, M., **Banerjee, A.,** Ignatova, N., Föhlisch, A., Gel'mukhanov, F. and Kimberg, V. *J. Chem. Phys. 159,* **2023**. *(Just accepted)*

Other Projects from the Postdoctoral research carried out at Fysikum, Stockholm University with Prof. Michael Odelius are being extended onto Uppsala University where I am currently employed under the supervision of Prof. Philippe Wernet, with three manuscripts under preparation and two other projects in advanced stage of completion.

Weizmann Institute of Science

10. Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: Hückel-Möbius Interconversions in Expanded Porphyrins, Sylvetsky, N., † **Banerjee, A**., † Alonso, M., & Martin, J. M. L. [† as equal 1st author] *Journal of Chemical Theory and Computation. 16,* **2020**, *3641–3653*

11. Performance of Electronic Structure Methods for the Description of Hückel-Möbius Interconversions in Extended π-Systems. Woller, T., **Banerjee, A.**, Sylvetsky, N., Santra, G., Deraet, X., De Proft, F., Martin, J. M. L. & Alonso, M. *The Journal of Physical Chemistry A, 124,* ***2020****, 2380-2397*

Indian Association for the Cultivation of Science

12. Theoretical investigations on the mechanistic aspects of O_2 activation by a biomimetic Dinitrosyl Iron complex. **Banerjee, A.,** Sen, S., Paul, A., *Chemistry–A European Journal, 24,* **2018**. 3330-3339. (Selected for HOT PAPER)

13. Deciphering the cryptic role of catalytic electron in a photochemical bond dissociation using Aromaticity markers. **Banerjee, A**., Halder, D., Ganguly, G. and Paul, A. *Phys. Chem. Chem. Phys*., 18, **2016**, 25308-25314.

14. A Serendipitous Rendezvous with a Four-Center Two-Electron Bonded Intermediate in the Aerial Oxidation of Hydrazine. **Banerjee, A**., Ganguly, G., Roy, L., Pathak, S., and Paul, A. *Chemistry–A European Journal,* 22, **2016**, 1216-1222. (Communication selected for frontispiece)

15. Unearthing the Mechanism of Prebiotic Nitrile Bond Reduction in Hydrogen Cyanide through a Curious Association of Two Molecular Radical Anions. **Banerjee, A**.,* Ganguly, G., Tripathi, R., Nair, N. N., and Paul, A. *Chemistry-A European Journal,* 20 **2014**, 6348-6357. (*as corresponding author)

16. Understanding the unexpected product distribution in the aerial oxidation of carbene stabilized diphosphorous complex. Ghosh, B.,† **Banerjee, A.,** † Paul, A., *Chemistry–A European Journal, 24,* **2018**. 4350-4360. [† as equal 1st author]

17. Ammonia–Borane Dehydrogenation by Means of an Unexpected Pentacoordinate Boron Species: Insights from Density Functional and Molecular Dynamics Studies. Bhunya, S.,† **Banerjee, A**.,† Tripathi, R., Nair, N. N., and Paul, A. *Chemistry-A European Journal,* 19, **2013**, 17673-17678. [† as equal 1st author]

18. Understanding the Role of Solvents and Spin–Orbit Coupling in an Oxygen-Assisted SN2-Type Oxidative Transmetalation Reaction. Ghosh, B., **Banerjee, A.**, & Paul, A., *Chemistry–A European Journal*, *25*, **2019**, 16606-16616.

19. Exploring the Crucial Role of Solvation on the Viability of Sustainable Hydrogen Storage in BN-fullerene: A Combined DFT and Ab initio Molecular Dynamics investigation. Ganguly G., Halder D., **Banerjee A**., Basu S., Paul A., *ACS Sustainable Chemistry & Engineering,* 7, **2019**, 9808-9821

20. Unraveling the Microscopic Origin of Triplet Lasing from Organic Solids. Paul, L., **Banerjee, A.**, Paul, A., Ruud, K., Chakrabarti, S., *J. Phys. Chem. Lett.*, 9, **2018**, 4314–4318.

21. Hydrogen-Bonding Directed Assembly and Gelation of Donor–Acceptor Chromophores: Supramolecular Reorganization from a Charge-Transfer State to a Self-Sorted State. Das, A., Molla, M. R., **Banerjee, A.**, Paul, A., and Ghosh, S. *Chemistry-A European Journal,* 17, **2011**, 6061-6066. .(Back cover Article)

22. Benzimidazole Linked Arylimide Based Covalent Organic Framework as Gas Adsorbing and Electrode Materials for Supercapacitor Application. Roy, A., Mondal, S., Halder, A., **Banerjee, A.**, Ghosal, D., Paul, A., Malik, S. *European Polymer Journal*, **2017**, DOI: 10.1016/j.eurpolymj.2017.06.028

Research Expertise

Level of Research	Reaction mechanism	Excited-state MD	Solvent phase MD	Time-resolved spectroscopy	Benchmark studies
PhD IACS(Kolkata)	DFT NEVPT2/CASPT2	CASSCF Surface-hopping	DFT CPMD		
PDF1 (1 year) Weizmann Inst.					DLPNO-CCSD(T)
PDF2 (2 years) Stockholm Uni.	DFT NEVPT2/CASPT2	CASSCF/TDDFT Surface-hopping	DFT CPMD/CP2K	XAS, RIXS, XPS, XES	
PDF3 (1year ---) Uppsala Uni.	DFT NEVPT2/CASPT2	CASSCF/TDDFT Surface-Hoping		XAS, RIXS, XPS, XES	

Scientific interests for future research

- Elucidation of excited state process and reaction dynamics in molecular systems. These include photochemistry and ultrafast dynamics in transition metal complexes and organic molecules which can unravel important aspects of fundamental photochemistry and photo-physics. Use of novel surface hopping excited state dynamics and MCTDH (based on LVC models) techniques to study ultra-fast dynamics in photo-physical processes.
- Theoretical modelling of various time resolved spectroscopic techniques and predicting systems that can be studied using them.
- Application of state-of-the-art multi-reference quantum chemical techniques to novel chemical reaction pathways.
- Charting out chemical reaction mechanisms for ground state reactions which are often extremely useful to experimental organic and inorganic chemists.
- Simulation and understanding of X-Ray spectroscopic observables like from XAS/RIXS/XPS/XES experiments with the state-of-art electronic structure methods.
- Active member in various collaborations at different short pulse X-Ray facilities [LCLS(USA) & SwissFEL(Switzerland) X-Ray lasers and BESSY(Germany) SLS(Switzerland) & SSRL(USA) synchrotrons]
- Development of newer protocol to study core-level spectroscopies for larger systems including ones in condensed phase.
- Spin forbidden reactions, and role of Spin-Orbit Coupling in them.
- Wavepacket dynamics

- Benchmarking studies of different quantum chemical methods and developing benchmark data sets for calibrating newly developed theories.

Education

Doctor of Philosophy in Chemistry (Physical Chemistry)

- Indian Association for the Cultivation of Science, Kolkata, WB, India, 2017.
- Thesis Title: Probing Aromaticity in Intermediates and Transition States along Non-Traditional Reaction Paths.
- Adviser: Prof. Ankan Paul
- Area of Study: Elucidation of ground and excited state reaction mechanism using static quantum chemical techniques (DFT, CASSCF, MRPT2 (techniques), CCSD, MP2, etc.) and Molecular Dynamics.
- Key Courses: Advanced Quantum Mechanics, Group Theory, Advanced Quantum Chemistry.

Master of Science in Chemistry (Physical Chemistry)

- **University of Calcutta, Calcutta, WB, India, 2008-2010**
- **Specialization: Physical Chemistry**
- **Class/Division: 1st class**

Bachelor of Science in Chemistry (Hons.)

- **University of Calcutta, Calcutta, WB, India, 2005-2008**
- **Class/Division: 1st class (67.5%)**
- Major: Chemistry (with Hons) ; Minor: Mathematics, Physics

Academic Honours and Award

- Dean's Postdoctoral Fellowship, Weizmann Institute of Science, Israel.
- National Eligibility Test (CSIR/UGC NET, India) Dec-2009 (Junior Research Fellowship, Senior Research Fellowship (2012)
- Graduate Aptitude Test in Engineering (GATE-Chemistry) 2010.
- Best Poster Award at In house Symposium for National Science Day Celebration at IACS 2014.

Skills

- Well versed in carrying out excited state MD modelling of photo-chemical/photo-physical processes.
- Experienced with tracing out complex reaction mechanisms both in ground and excited state.

- Molecular Dynamics (BOMD and CPMD)
- Experienced with DFT (choice of functional at different scenarios) and bench marking them.
- Application of CASSCF and Multireference Perturbation (NEVPT2/SS-MRPT2/MRCPT2) techniques to chemical processes. (Making proper choice of active space and theoretical knowledge of Multireference Perturbation Theories)
- Aromaticity quantifies. MICD (magnetically induced current density as implemented in DALTON), NICS (CASSCF, DFT and MP2 level)

References

- **Prof. Michael Odelius**

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- **Prof. Philippe Wernet**

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