

*Ms. Suhita Basumallick*

*Research Associate*

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## *Academic Qualifications*

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2009-2012	B.Sc. in Chemistry, Lady Brabourne College, University of Calcutta (CU).
2012-2014	M.Sc. in Chemistry, University of Calcutta (CU).
June 2015	Qualify National Eligibility Test (NET), Rank: CSIR-28.
December 2015 to July 2021	Ph.D. in Quantum chemistry under the supervision of <b>Prof. Sourav Pal</b> , Indian Institute of Technology Bombay (IITB).
September 2021 to Present	Post-Doctoral Research Associate under the supervision of <b>Prof. Piotr Piecuch</b> , Michigan State University (MSU).

## *Research Interests*

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My main research goal is the development of formulations capable of generating the effects of higher-rank excitations needed for a quantitative account of the electron correlation in molecular systems plagued with quasi-degeneracy and the application of those tools to the studies of metastable states of molecules, which can be elegantly dealt with by a correlated independent particle approximation to CAP-FSCC. I have gained expertise in quantum chemistry coding especially in blossoming of accurate, computationally efficient and least expensive partial fourth order schemes of (0,1), (1,0), (1,1) sectors within FS-MRCC, capable of generating the effects of triple, based on the non-iterative, perturbative philosophies.

## *Publications*

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1. 2020 Suhita Basumallick, Sumantra Bhattacharya, Irina Jana, Nayana Vaval, Sourav Pal. Shape resonance of sulfur dioxide anion excited states using CAP-CIPFSMRCCSD method. *Mol. Phys.* 2020, **118** (16), 1-8.

2. 2020 Suhita Basumallick, Sourav Pal, M. V. Putz. Fock-Space Coupled Cluster Theory: Systematic Study of Partial Fourth Order Triples Schemes for Ionization Potential and Comparison with Bondonic Formalism. *Int. J. Mol. Sci.* 2020, **21**, 6199.
3. 2020 Suhita Basumallick, Y. Sajeev, Sourav Pal. Nayana Vaval. Negative Ion Resonance States: The Fock-Space Coupled-Cluster Way. *J. Phys. Chem. A.* 2020, **124** (50), 10407-10421.
4. 2021 Irina Jana, Suhita Basumallick, Sourav Pal, Nayana Vaval. Resonance Study: effect of partial triples excitation using CAP-based Fock-space multi-reference coupled cluster. *Int. J. Quantum Chem.* 2021, **121**, e26738.
5. 2021 Suhita Basumallick, M. V. Putz, Sourav Pal. Three-Body Excitations in Fock Space Coupled-Cluster: Fourth Order Perturbation Correction to Electron Affinity. *Int. J. Mol. Sci.* 2021, **22**, 8953.
6. 2021 Suhita Basumallick, Sourav Pal. Partial fourth order schemes of triples in Fock space coupled-cluster theory: Ionization potentials of Ozone. *Journal of the Indian Chemical Society.* 2021, **98**, 100166.

### *Conference Presentations*

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- February 2019 Suhita Basumallick, Sumantra Bhattacharya, Irina Jana, Nayana Vaval and Sourav Pal. ***“Correlated Complex Independent Particle Theory In FSMRCC: Application To The Shape Resonance Of Sulfur Dioxide Anion Excited States.”*** Theoretical Chemistry Symposium (TCS), BITS Pilani, India.
- September 2019 Suhita Basumallick, Sourav Pal. ***“Three Body Excitation Effect In Fock Space Coupled Cluster: Fourth Order Perturbation Correction To Electron Affinity.”*** Current Trends in Theoretical Chemistry VIII (CTTC VIII), Kraków, Poland.

### *Awards*

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- 01.01.2016 to 30.12.2020 Council of Scientific & Industrial Research (CSIR) Fellowship.

### *Experience*

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2018 & 2019      Work as a Teaching Assistant in UG lab course (CH 117L) at IITB.

25.01.2021 to  
06.07.2021      Work as a Research Associate at IITB.

## *References*

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Prof. Sourav Pal      Director, Indian Institute of Science Education and Research Kolkata,  
Mohanpur, Nadia 741246, West Bengal, India.  
Former HAG and Institute Chair Professor, IIT Bombay, India.  
Former Director, CSIR -NCL, Pune, India.  
Email: s.pal@iiserkol.ac.in.

Prof. Nayana Vaval      Faculty of CSIR-National Chemical Laboratory,  
Dr. Homi Bhabha Road, Pune-411008, India.  
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