Atanu Maity, Ph.D.

Postdoctoral Fellow
Department of Chemistry, IIT Bombay
Powai, Mumbai-400076

Gender: Male | **Marital Status:** Single
Nationality: Indian | **D.O.B.:** September 7, 1988
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Area of Specialization:
Computational Biophysics, Computational Chemistry, Statistical mechanics

Research Experience

July, 2018 - present	**Postdoctoral Fellow**, *Dept. of Chemistry, IIT Bombay, Mumbai, India.* Supervisor: Dr. Rajarshi Chakrabarti
Feb, 2018 - July, 2018	**Research Assistant,** *Bioinformatics centre, Bose Institute, Kolkata, India*
Aug, 2013 - Feb, 2018	**Senior Research Fellow,** *Bioinformatics centre, Bose Institute, Kolkata, India*
Aug, 2011 - Aug, 2013	**Junior Research Fellow,** *Bioinformatics centre, Bose Institute, Kolkata, India*

Educational Qualification

Aug, 2011 - Aug, 2017	**Ph. D.**, *Calcutta University, India (Work place: Bose Institute)* Thesis Title: Flexibility and conformational modulations of proteins correlating apoptosis: Molecular Dynamics simulations of Bcl2 family members Supervisor: Dr. Shubhra Ghosh Dastidar
2009 - 2011	**M. Sc.(Chemistry),** *Vidyasagar University, W.B., India* 61.5 % | Specialization: Physical Chemistry
2006 - 2009	**B. Sc.(Chemistry),** *Tamralipta Mahavidyalaya, W.B., India* 60.5 % | Major: Chemistry | Minors: Physics, Mathematics

Fellowships and Awards

2018	Awarded **Institute Postdoctoral Fellowship**, *IIT Bombay, Mumbai, India.*
2013	Awarded **Senior Research Fellowship,** *CSIR, Govt. of India*
2011	Awarded **Junior Research Fellowship,** *CSIR, Govt. of India*
2011	Qualified **National Eligibility Test for research and lectureship,** Chemical Science
2011	Qualified **Graduate Aptitude Test,** Chemical Science

Skills and Expertise

- Modelling Biomolecular assemblies and their interactions at atomic level
- Conformational sampling and statistical analysis using MD simulation
- Protein-protein and protein-ligand binding free energy calculations using MMGBSA methods
- Free energy calculation of biomolecular transformations from enhanced sampling (PMF)
- Identifying functional modes of proteins using PCA

Publications

- **Maity, A.**, Sarkar, S., Theeyancheri, L., & Chakrabarti, R. (2019). Choline chloride as a nano-crowder protects HP-36 from urea-induced denaturation: Insights from Solvent Dynamics and Protein-Solvent interaction. *arXiv preprint* arXiv:1909.06757.
- **Maity, A.**†, Sinha, S.†, & Dastidar, S. G. (2019). Dissecting the thermodynamic contributions of the charged residues in the membrane anchoring of Bcl-xl C-terminal domain. Chem. Phys. Lipids., 218, 112-124.
- Sarkar, S., **Maity, A.**, Sarma Phukon, A., Ghosh, S., & Chakrabarti, R. (2018). Salt Induced Structural Collapse, Swelling, and Signature of Aggregation of Two ssDNA Strands: Insights from Molecular Dynamics Simulation. The J. Phys. Chem. B, 123(1), 47-56.
- **Maity, A.**, Majumdar, S., & Dastidar, S. G. (2018). Flexibility enables to discriminate between ligands: Lessons from structural ensembles of Bcl-xl and Mcl-1. Comput. Biol. Chem., 77, 17-27.
- Sinha S.†, **Maity, A.**, & Ghosh Dastidar, S. (2017). BIM Binding Remotely Regulates BAX Activation: Insights from the Free Energy Landscapes. J Chem Inf Model, Just Accepted Manuscript DOI: 10.1021/acs.jcim.7b00628
- Priya, P., **Maity, A.**, & Ghosh Dastidar, S. (2017). The long unstructured region of Bcl-xl modulates its structural dynamics. Proteins, 85(8), 1567-1579.
- **Maity, A.**†, Sinha, S.†, Ganguly, D., & Ghosh Dastidar, S. (2016). C-terminal tail insertion of Bcl-xL in membrane occurs via partial unfolding and refolding cycle associating microsolvation. Phys. Chem. Chem. Phys., 18(34), 24095-24105.
- Priya, P., **Maity, A.**, Majumdar, S., & Ghosh Dastidar, S. (2015). Interactions between Bcl-xl and its inhibitors: Insights into ligand design from molecular dynamics simulation. J Mol Graph Model, 59, 1-13.
- **Maity, A.**†, Majumdar, S.†, Priya, P., De, P., Saha, S., & Ghosh Dastidar, S. (2015). Adaptability in protein structures: structural dynamics and implications in ligand design. J. Biomol. Struct. Dyn., 33(2), 298-321.
- Bhar, K.†, **Maity, A.**†, Ghosh, A.†, Das, T., Dastidar, S. G., & Siddhanta, A. (2015). Phosphorylation of Leghemoglobin at S45 is Most Effective to Disrupt the Molecular Environment of Its Oxygen Binding Pocket. Protein J., 34(2), 158-167.
- **Maity, A.**, Yadav, S., Verma, C. S., & Ghosh Dastidar, S. (2013). Dynamics of Bcl-xL in water and membrane: molecular simulations. PLoS One, 8(10), e76837.

† Equally contributed

Conference and Workshop

- Summer School on Rare Event Sampling, organized by University of Ilinois and Indian Institute of Science, Bengaluru, India, July(2019). †
- *Dynamics at The Interface Of Chemistry And Biology,* organized by: Indian Institute of Science held at Bangalore, India, Feb 18-20th (2019). †
- *3rd National Postdoctoral Symposium,* organized by: National Centre for Biological Science and Centre for Cellular and Molecular Biology at Hyderabad, India, Oct 3-5th (2018). ≠
- *Third International symposium on protein folding and dynamics*, organized by: National Center of Biological Science held at Bangalore, India, Nov 8-11th (2016) .†
- *Conference on Informatics & Integrative Biology*, organized by: Centre for Bioinformatics, Bose Institute held at Bose institute, Kolkata, India, Dec 17-19th (2014) .

- *International Conference on "Biomolecular Forms and Functions"* organized by: Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, Jan 8 – 11th (2013). †
- *Theoretical Chemistry Symposium*, organized by: Department of chemistry, IIT Guwahati, India, Dec 19-22nd (2012) †.
- *Conference on Informatics & Integrative Biology*, organized by: Centre for Bioinformatics, Bose Institute held at Bose institute, Kolkata, India, Dec 17-19th (2011).

† Poster presentation, ≠ Oral presentation

Computational Expertise

- MODELLER and SWISS-MODEL (webtools) for homology modelling
- Haddock (webtools) for protein-protein and protein-nucleic acid docking
- CHARMM, NAMD and GROMACS for MD simulation
- Enhanced sampling techniques (Adaptive Biasing Force methods, Umbrella sampling, Metadynamics)
- Gaussian for QM calculation
- Clustal Omega for multiple protein sequence analysis
- Pymol, VMD, Chimera, Bio3D (R) for visualization and structural analysis
- Linux operating system and shell scripting
- Parallel computing in HPC with Job scheduling in CRAY architecture
- FORTRAN, Python programming language

References

Dr. Shubhra Ghosh Dastidar

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