Resume

Dr.Timir Hajari, M.Sc., Ph.D.

❖ Personal Details

Sex: Male
Date of Birth: 19/03/1989
Nationality: Indian

Address:
Vill. – Rasulpur, P.O. – Jangalpara,
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❖ Current Position: **Assistant Professor (Stage 1), Department of Chemistry, City College, 102/1 Raja Rammohan Sarani, Kolkata-700009. (Under Calcutta University).**

❖ Educational qualifications:

Course	University
B.Sc. (Chemistry, Hons.), 2009	Ramakrishna Mission Vidyamandira, (under University of Calcutta)
M.Sc.in Chemistry, 2011	Indian Institute of Technology Bombay, Mumbai, Maharashtra
Ph.D., Physical Chemistry 2015	TU-Darmstadt, Germany
Post Doct. , Physical Chemistry , 2017	Indian Institute of Technology Kharagpur, West Bengal

❖ Technical, workshop & Academic Training :

Faculty Induction Programme/ Orientation Programme (Online), 2023, Kannur University, HRDC

❖ Previous working experience:

Sl. No.	Post	College, University and Organisation	Department	Duration
1	Assistant Professor	Heritage Institute of Technology, Kolkata	Chemistry	2017-2020
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❖ Area of expertise and Research Interest:

I am a Computational Physical Chemist. My research interest is related to solvation thermodynamics. Computer Simulations are used on these regards. My research interests are :

- Molecular simulations of bio-molecules
- Water structure around hydrophobic and hydrophilic groups
- Effect of ions and osmolytes on protein/DNA/polymer conformations
- Ion-pairing in aqueous solution.

❖ Publication:

Papers:

Impact of an Ionic Liquid on Amino Acid Side Chains: A Perspective from Molecular Simulation Studies, K. P. Ghanta, S. Mondal, T. Hajari, S. Bandyopadhyay, ***Journal of Chemical Information and Modeling*** 63 (2023), 959.

Hydrophobic association and solvation of neopentane in urea, TMAO and urea–TMAO solutions, T. Hajari, M. Dixit, H. O. S. Yadav, ***Physical Chemistry Chemical Physics*** 24 (2022), 6941.

Ion pairing and preferential solvation of butylmethylimidazolium chloride ion pair in water-ethanol mixtures by using molecular dynamics simulations, M. D. Meti, M. Dixit, T. Hajari, B. L. Tembe, ***Chemical Physics Letters*** 720 (2019), 107.

Water structure around hydrophobic amino acid side chain analogs using different water models, T. Hajari, S. Bandyopadhyay, ***The Journal of Chemical Physics*** 146 (2017), 225104.

Solvation structures of sodium halides in dimethyl sulfoxide (DMSO)–methanol (MeOH) mixtures, M. K. Dixit, T. Hajari, B. L. Tembe, ***Molecular Simulation*** 43 (2017), 154.

The effect of urea and taurine osmolytes on hydrophobic association and solvation of methane and neopentane molecules, M. K. Dixit, T. Hajari, B. L. Tembe, ***Journal of Molecular Liquids*** 223 (2016), 660.

Mechanism of polymer collapse in miscible good solvents, F. Rodríguez-Ropero, T. Hajari, N. F. A. van der Vegt, ***The Journal of Physical Chemistry B*** 119 (2015), 15780.

Solvation thermodynamics of amino acid side chains on a short peptide backbone, T. Hajari, N. F. A. van der Vegt, ***The Journal of chemical physics*** 142 (2015), 04B607.

Mutual exclusion of urea and trimethylamine N-oxide from amino acids in mixed solvent environment, P. Ganguly, T. Hajari, J. E. Shea, N. F. A. van der Vegt, ***The journal of physical chemistry letters*** 6 (2015), 581.

Peptide backbone effect on hydration free energies of amino acid side chains, T. Hajari, N. F. A. van der Vegt, ***The Journal of Physical Chemistry B*** 118 (2014), 13162.

Molecular Simulation Study on Hofmeister Cations and the Aqueous Solubility of Benzene, P. Ganguly, T. Hajari, N. F. A. van der Vegt, ***The Journal of Physical Chemistry B*** 118 (2014), 5331.

Enthalpy–entropy of cation association with the acetate anion in water, T. Hajari, P. Ganguly, N. F. A. van der Vegt, ***Journal of chemical theory and computation*** 8 (2012), 3804.

Potentials of mean force for the exo and endo solvolysis of 2-norbornyl chloride in water and DMSO: A constrained molecular dynamics study, S. C. Tiwari, T. Hajari, A. Sharma, B. L. Tembe, ***Journal of Chemical Sciences*** 124 (2012), 327.

❖ List of Participation in Seminar, Conference and Workshop

- Presented poster at the *Theoretical Chemistry* Symposium (December 14-17 *2016*) at University of *Hyderabad.*
- Poster presentation on Bunsentagung 2015 – 114th General Assembly of the German Bunsen Society for Physical Chemistry.
- Poster presentation at CECAM workshops May 14, 2014 to May 17, 2014 "Entropy in Biomolecular Systems"
- Talk and Poster presentation at the Workshop in Hünfeld, April 11-12, 2014 "Computer simulation and theory of macromolecules 2014"

❖ Additional activities:

Resource Person at Faculty Development Programme (5^{th} June to 11^{th} June, 2023) on Computer Programming Basics (Fortran) Organized by Department of Chemistry, The Bhawanipur Educational Society College.