CURRICULUM VITAE/RESUME

Arijit Mondal

Post-Doctoral Research Fellow(IISER-T)

Ph.D. in Physics (Awarded on 14th Feb. 2020)
Jawaharlal Nehru University, New Delhi-110067

Personal Details:

Date of Birth: **02/04/1990** **Sex:** **Male**

Category: **EWS(Economically Weaker Section under General Caste)**

Father's name: Ashok Mondal Mother's name: Rita Mondal

Nationality: Indian Languages: Bengali, English, Hindi

Domicile: West Bengal

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Career Objective:

To work hard and facilitate the process of self-enrichment and to give my best to the institution, where I work. To channelize my energies in a positive direction and to deliver the best possible service I can give.

Doctoral Degree Details:

Field: Theoretical and Computational Statistical Physics.

Thesis Title-**Configurational Entropy and Fragility of soft matter: A common basis using microscopic models.**

Thesis Supervisor**:** Prof. Shankar Prasad Das

Ph.D. Registration Date/Joining Date: 08/08/2013

Ph.D. Thesis Submission Date: 04/07/2019

Ph.D. Thesis Defense Date: - 14/02/2020

Ph.D. Award Date: -14/02/2020

Education:

Examination Passed	Board/University	Year of Passing	Total Marks	Marks Obtained	% of Marks /Grade	Class /Division	Subject Studied
Ph.D.	Jawaharlal Nehru University						
M.Sc.	Visva-Bharati University	2012	1200	738	61.50	1st	Physics
B. Sc.	University of Burdwan	2010	800	473	59.12	2nd	Phy.(H), Math.(S),Chem(S)
Higher Secondary	S.S,A. Institution	2007	500	370	74*	1st	Beng. Eng. Math, Phy., Chem., Bio.(S)
Secondary	S.S,A. Institution	2005	800	624	78	1st	Math., P.Sc., L.Sc, Eng., Beng. Hist., Geo.

***Without Counting Additional**

Summary of Research Work During Ph.D.:

In my Ph.D., I worked on glass Systems by using the classical density functional theory (DFT**)** approach. We evaluated the free energy of a hard-sphere amorphous system by using classical DFT. In classical DFT there are two standard methods of computing the free energy of inhomogeneous system-Ramakrishnan-Yusuff free energy functional approach (RY) and the

modified weighted density functional approach (MWDA). We extended this classical DFT by computing the configurational entropy. The configurational entropy is defined as the difference between the total entropy and the vibrational entropy of the system. Here we used MWDA approximation to evaluate the total free energy (or the total entropy) of the hard-sphere system. We observed that the configurational entropy depends upon the amorphous structure**.** This work has been **published** in Phys. Rev. E.

In our next project, we studied the free energy and configurational entropy for a soft inverse-n power potential system, where n approaches to ∞ is the hard-sphere limit. Using the Barker-Henderson integral, we mapped the soft-sphere system with diameter $\boldsymbol{\sigma}$ to a hard-sphere system with a properly chosen diameter(d) and estimate the free energy and the configurational entropy by using MWDA. The dynamics of the system is quantified by the term fragility which is the slope of the relaxation time with the volume fraction scaled with the glass transition volume fraction. We computed the fragility of our system by linking thermodynamic quantity configurational entropy with dynamic quantity relaxation time through the Adam-Gibbs relation. In our work, the fragility was estimated from the thermodynamic term configurational entropy, therefore, termed as Thermodynamic fragility. We solved the Mountain-Zwangig(MZ) equations of high-frequency elastic modulus (shear-modulus and Bulk modulus) and numerically estimated the high-frequency elastic modulus of the aforementioned interacting potential system. The elastic response of the system is described by the term Poisson's ratio or the ratio of shear-modulus and Bulk modulus. In this work, a link between static elastic quantity Poisson's ratio with thermodynamic fragility was established (this work has been **published** in an international Journal (PTEP)).

In our third project, we studied the elastic and dynamic properties of soft colloids. from the experimental data of Mattson. et. al. (Nature 462, page 83). Here we computed the elastic energy theoretically by using the MZ equation. After fitting our theoretical data with their experimental data we computed the steepness parameter and strength of interaction potential when it has the inverse-n form. We have also done the same by using Hertzian potential as an interparticle interaction potential, where the strength and diameter of the system have been taken as mapping parameters. Then by using these mapping parameters the high-frequency elastic properties of soft-colloids had been studied. A link between dynamics to elasticity for these colloid systems has been established later (this work has been **published** in an international Journal (CMP)).

Summary of Research Work Doing in First Post-Doc.:

In Post-Doc. Currently, I am working with super-cooled water. We have done NPT molecular dynamic simulation by using GROMACS and generated the equilibrium real dynamical configuration of TIP4P/2005 water model. After minimizing this real dynamical configuration, we generate the inherent structure of the system. This inherent structure is the equilibrium structure in

the potential energy surface. We are trying to explore the thermodynamic anomalies hidden in the path of the potential energy surface. We are currently preparing the **manuscript** of this work.

Publications:

Journal Publications:

(1) Dependence of the configurational entropy on amorphous structures of a hard-sphere fluid.

Arijit Mondal, Leishangthem Premkumar, and Shankar P. Das
Phys. Rev. E **96,** 012124(2017)

https://doi.org/10.1103/PhysRevE.96.012124

(2) A classical density functional theory model for fragility in the hard-sphere limit.

Arijit Mondal, and Shankar P. Das

Progress of Theoretical and Experimental Physics **2020**(7), 073I02(2020)

https://doi.org/10.1093/ptep/ptaa091

(3) Configurational entropy of a parabolic potential system: A density functional approach.

Arijit Mondal

Phys. Scr. **96**,025703(2020)
https://doi.org/10.1088/1402-4896/abce76

(4) Correlation between kinetic fragility and Poisson's ratio from analysis of data for soft colloids.
Arijit Mondal, Leishangthem Premkumar, and Shankar P. Das
Condensed Matter Physics 24, 13602(2021)
https://doi.org/10.5488/CMP.24.13602

Under Construction:

(5) Structural origin of thermodynamic anomalies of supercooled water

Arijit Mondal, Gadha R., and Rakesh S. Singh

Conference Publication:

(6) Configurational entropy of a hard sphere system using Modified Density Functional Approximation(MWDA)
Arijit Mondal, Leishangthem Premkumar, and Shankar P. Das
AIP Conference Proceedings **2115**, 030227 (2019)
DOI:10.1063/1.5113066

Achievements/Awards/Other Qualifications:

Exam. Qualified	Year	All India Rank
CSIR-UGC National Eligibility Test (NET)	Dec.2017	Lectureship-25
JEST	2019	304
GATE	2017	187
JAM	2012	206

Seminars/Conferences attended:

1. Poster presentation and a conference proceeding at DAE conference. Date:18th Dec. 2018.
2. Bangalore School of Statistical Physics. Date:2nd June 2015 to 18th June 2015.

Teaching Assistantship:

1. Advanced Statistical Physics course (2015) at JNU.
2. Non-equilibrium Statistical Physics course (2021) at IISER-T
3. Computer application course using Python (2022) at IISER-T

Computational/Technical skills:

- **Programming Language:** Fortran, C, Python
- Work experience on utilities like Grace, Gnuplot, Latex etc.

- **System Software:** Windows, Linux Mint, Ubuntu, Elementary Os, Zorin 9, Pippermint Os.
- **Application software:** Microsoft Office, Notepad++, Microsoft Excel. Powerpoint
- **Simulation Tools:** Knowledge of Monte Carlo and Molecular Dynamics simulation
- **Simulation Software:** Knowledge of GROMACS, and LAMMPS

References:

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School of Physical Sciences,

Jawaharlal Nehru University

Email: shankar0359@yahoo.com

(2) Prof. Swapan Mandal

Dept. of Physics,

Visva-Bharati University

Email: swapanvb@rediffmail.com

Date: 02.05.2022

Place: West Bengal, India

Signature