

TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO ID CODE: 5854

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Dipartimento di Fisica Aldo Pontremoli**

Scientist- in - charge: Prof. Alessio Zaccone

[Name and surname]

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	SINGH
Name	ANKIT

PRESENT OCCUPATION

Appointment	Structure
Research Scholar (PhD)	Banaras Hindu University, Varanasi-221005, India

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
PhD	Physics	BHU, Varanasi, India	Thesis submitted June 2023
Master	Physics	UP College, Varanasi, Mahatma Gandhi Kashi Vidyapith University, Varanasi	2015 (77.50%)
Bachelor	Physics, Chemistry, Mathematics	UP College, Varanasi, Mahatma Gandhi Kashi Vidyapith University, Varanasi	2012 (70.44%)

REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of Association City

Università degli Studi di Milano – Direzione Trattamenti Economici e Lavoro Autonomo Ufficio Contratti di formazione e Ricerca Via Sant'Antonio 12 - 20122 Milano, Italia <u>assegni.ricerca@unimi.it</u> DTELA_M_CVAssegniENG_rev. 00 del 02/09/2021



FOREIGN LANGUAGES

Languages	level of knowledge
Hindi	Mother tongue
English	Fluency

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2016	Graduate Aptitude Test in Enginnering (GATE) cunducted IISC Bangalore
2016	National Eligiblity Test (CSIR-NET-JRF) in Physical Sciences
2017	GATE cunducted IIT Roorke
2018	Award of CSIR Research Fellowship for PhD
2018-20	CSIR Junior Research Fellowship
2020-23	CSIR Senoir Research Fellowship

TRAINING OR RESEARCH ACTIVITY

Ph.D in Physics under supervision of Prof. Yashwant Singh (thesis submitted)

Title: Structural ordering and super-Arrhenius dynamics of glass-forming liquids

During my Ph.D., we developed a theory to calculate the structural relaxation time. Our theory identifies the local structural order that defines the cooperativity of relaxation and reveals several underlying features of the activated dynamics of glass formers. We explored collective behavior, cooperative correlation length scales, and the identification of local structural orders that govern the cooperativity of relaxation. Our work provides a first-principle theory to calculate the "cooperative reorganizing cluster" and the super-Arrhenius dynamics of glass formers.

we investigated the super-Arrhenius behavior of structural transition in monodisperse hard spheres and binary mixture of hard sphers. The potential barrier height is shown to increase due to an increase in the number of the 'stable bonds' a particle forms with its neighbors and the energy of each bond as liquids move deeper into the supercooled (supercompressed) region. We presented results for a system of hard spheres and compare calculated values of the structural relaxation time with experimental and simulation results.

we investigated the structure and activated dynamics of a binary mixture of colloidal particles dispersed in a solvent of much smaller-sized particles. The solvent can be used as a control parameter to fine-tune the microscopic structural ordering of colloidal particles and, therefore, the emergence and the size of CRC that governs the glassy dynamics. Our findings suggest that a small variation in the concentration of solvent can create a bigger change in the kinetic fragility in the hard-sphere colloidal systems which highlights a wide variation in behavior, ranging from fragile to strong glasses.

we have calculated the structural relaxation time τ_{α} of fragile supercooled liquids. Using the information of the configurational entropy and structure, we calculate the number of



dynamically free, metastable, and stable neighbors around a central particle. Our theory brings forth a temperature Ta and a temperature dependent parameter $\psi(T)$ which characterize slowing down of dynamics on cooling. We present results for the Kob-Anderson model for three densities and show that the calculated values of $\tau \alpha$ are in excellent agreement with simulation values for all densities. We also show that when $\psi(T)$, $\tau \alpha$ and other quantities are plotted as a function of rescaled temperature T/T_a (or T_a/T) the data collapse on master curves.

we investigated the dependence of slowing down of dynamics of glass-forming liquids on the attractive and repulsive parts of intermolecular interactions. Through an extensive comparison of the behavior of a Lennard-Jones glass-forming liquid and that of its WCA reduction to a model with truncated pair potential without an attractive tail we demonstrate why the two systems exhibit very different dynamics despite having nearly identical static correlation functions. In particular, it is shown that the local structures are characterized by a number of mobile and immobile particles around a central particle that markedly differ in the two systems at densities and temperatures where their dynamics show large differences and identical when structures nearly overlap.

We also investigated the kinetics of the collapse transition for a polymer of length *N* when a specific monomer is pinned using molecular dynamics simulations. We calculated the radius of gyration for the aggregate measurement of different polymer states and used them to calculate the collapse time (τ_c) for a pinned as well as free polymer, and the scaling behavior of (τ_c) with *N* is obtained.

Presently, we are extending our work to develop a theory for calculating the structure and relaxation time of hard spheres "quenched-annealed" (HS-QA) systems, as well as in a pinned glass-forming system. During my research period, I have published 05 research papers (+1 on arXiv+02 are under preparation) in reputed international journals and learned various simulation and theoretical techniques i.e. Density Functional Theory, Integral Equation Theory, Molecular Dynamic simulations.

PROJECT ACTIVITY

Year	Project
2016- 2023	PhD (Structural ordering and super-Arrhenius dynamics of glass-forming liquids)

PATENTS

Patent	

CONGRESSES AND SEMINARS

Date	Title	Place
July 12, 2023	Invited online talk titled 'Activated Dynamics of Glass-Forming Liquids' in the Soft Condensed Matter Theory Group by Prof. Dr. Klaus Kroy	Institute for Theoretical Physics, Leipzig University, Leipzig, Germany
March 17-	Workshop on Soft Matter: From	Banaras Hindu University Varanasi, India

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23, 2023	Physics to Biology	
Decembe r 11-16, 2022	flash talk and poster presentation titled 'Viscous slowing down of glass- forming liquids' in 5 th International Conference on Soft Materials	MNIT Jaipur, India
May 04- 06, 2022	Online Poster Presentation title 'Cooperativity and activated dynamics of supercooled liquids in a dense medium' in ICTP Hybrid Meeting on "Non-Markovian Dynamics Far From Equilibrium"	ICTP Italy, Trieste
February 14-20, 2020	Workshop on "DNA Bubble Formation: From Physics to Biological Functions"	BHU Varanasi, India
February 8th, 2020	"One Day Conference on Recent Trends in Research", (Poster Presentation).	BHU Varanasi, India
June 27 to 13 July 2018	"Bangalore School on Statistical Physics - IX"	ICTS Bangalore, India
May 2-15, 2017	Refresher course on "Statistical Mechanics and it's application",	Tripura University, Tripura, India
March 5-9 2019.	Workshop on "Fundamentals of Molecular Simulations"	Indian Institute of Technology, Kanpur, India
Septembe r 23-24, 2017	National Conference on "Current Trends in Physics"	BHU Varanasi, India
March 4, 2017	"10 th One-day Conference in Physics",	BHU Varanasi, India
March 17- 20, 2015	Workshop on " Light From Dark Side of the Universe"	BHU Varanasi, India

PUBLICATIONS

Books	
None	

Articles in reviews

A. Singh and Y. Singh, "Super-Arrhenius behavior of molecular glass formers", Phys. Rev. E Rapid Communications 99, 030101(R) (2019).

A. Singh, S. M. Bhattacharyya, and Y. Singh, "Emergence of cooperatively reorganizing cluster and super-Arrhenius dynamics of fragile supercooled liquids", Phys. Rev. E 103, 032611 (2021).

A. Singh and Y. Singh, "How attractive and repulsive interactions affect structure



ordering and dynamics of glass-forming liquids", Phys. Rev. E 103, 052105 (2021).

A. Singh and Y. Singh, "Structure ordering and glass transition in size-asymmetric ternary

mixtures of hard spheres: Variation from fragile to strong glasses", Phys. Rev. E 107, 014119 (2023).

K. Chauhan and A. Singh, "Delayed collapse transitions in a pinned polymer system",

Phys. Rev. E 105, 064505 (2022).

A. Singh and Y. Singh, "Understanding the phenomenon of viscous slowing down of glass-forming liquids from the static pair correlation function" arXiv:1909.02734 (2019).

A. Singh and Y. Singh, "Theory of activated glassy dynamics in a pinned supercooled liquids.", (Under preparation).

Congress proceedings

None

OTHER INFORMATION

Short term visit at NCL Pune Laboratory, Maharashtra, India from 16-30 January 2020.

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

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Place and date: Varanasi, India, 16/08/2023