

Dr. Inderdip Shere

Curriculum Vitae

MMS Lab, Chemical Engineering
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Research Interest

Designing efficient strategies to capture important molecular events accurately, which extends over various key areas such as, Molecular simulation, Monte Carlo techniques, Force-field development, Machine learning, Reaction kinetics, Multi-scale simulations, Self-assembly, Coarse-grain model development.

Current Position

10/2019-present **Research Associate**, *Chemical Engineering, IIT Bombay, Mumbai, India.*
Research theme: (a) Identification of reaction pathway in silica system, and (b) Development of reactive force-field for coarse grain silica species.
Supervisor: Prof. Ateeque Malani

Education

2012-19 **Ph.D. in Chemical Engineering**, *Indian Institute of Technology Bombay, Mumbai, India.*
2011-12 **Master of Chemical Engineering**, *Institute of Chemical Technology Matunga, Mumbai, India.*
2007-10 **Bachelor of Chemical Technology**, *Laxminarayan Institute of Technology, Nagpur, India.*

Ph.D. Thesis

Title Study of Silica Polymerization using Molecular Simulation Tools
Supervisor Prof. Ateeque Malani
Description The theme of this thesis is to understand the behavior of atomic species in manifesting macroscopic properties and developing various simulation strategies to efficiently capture these behaviors. Multi-scale simulation algorithms, based on the Monte Carlo approach, were designed to perform a poly-dimensional reaction of silica species. A coarse-grain model was also developed to study the more extensive system and explored various aspects of polymerization, such as the mechanism of reactions, phases of clusters, the kinetics of transformation, and polymerization stages. These studies established the relationship between the synthesis parameters with the products' final properties like size and shape of cluster, porosity, etc., which is crucial to design tailor-made materials. Overall this thesis provides a simulation approach from a molecular perspective useful to study any complex multi-functional reactive system.

Experience

2011 **In-plant Training**, IPCA LABORATORIES LIMITED, Ratlam, Madhya Pradesh.
Review of Environmental Compliance for IPCA Laboratories in Accordance to Madhya Pradesh Pollution Control Board, GOI
2009 **Summer Internship**, TATA MOTORS, Chinchwad, Maharashtra.
Reduction of Dust Defects in Vehicular Coating in Robotic Paint Shop.

Journal Publications

- [1] **Shere, I.** and Malani, A. *Porosity development in silica particles during self-assembly: Effect of solvent reactivity and precursor concentration.* **J Phys. Chem. C** 2020, 124, 520-530. <https://pubs.acs.org/doi/10.1021/acs.jpcc.9b08844>
- [2] **Shere, I.** and Malani, A. *Polymerization kinetics of a multi-functional silica precursor studied using a novel Monte Carlo simulation technique.* **Phys. Chem. Chem. Phys.** 2018, 20, 3554-3570. <https://pubs.rsc.org/en/content/articlehtml/2018/cp/c7cp07737h>

- [3] **Shere, I.** and Malani, A. *Formation and breaking kinetics of four and six member rings during the synthesis of silica nano-particles* (Manuscript in preparation).
- [4] **Shere, I.** and Malani, A. *Development of coarse-grain potential for silica species in aqueous medium* (Manuscript in preparation).

Research Presentations

- 2021 Inderdip Shere and Ateeque Malani, Poster presentation: *"Development of Coarse-Grain Silica Model to Study Nanoparticles Synthesis"*, Martini 3.0 online workshop, University of Groningen, Netherlands, 1-3 September.
- 2020 Inderdip Shere, Invited talk: *"Strategically Boosting Scales of Simulation: Development of the Coarse-Grain Model."*, Basic Principles of DFT Calculations & Molecular Dynamics Simulations (online), Malaviya National Institute of Technology, Jaipur, India, 23- 27 November.
- 2020 Inderdip Shere and Ateeque Malani, Poster presentation: *"Porosity Development in Silica Cluster During Self-Assembly: Effect of Solvent Reactivity and Precursor Concentration"*, Modern Approaches in Chemistry and Biology, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, India, 18 - 20 February.
- 2018 Inderdip Shere and Ateeque Malani, Oral presentation: *"How to Synthesize a Desired Polymeric Structure? A Molecular Simulation Perspective"*, CheMference, Indian Institute of Technology Bombay, Mumbai, India, 19 - 20 May.
- 2017 Inderdip Shere and Ateeque Malani, Oral presentation: *"Development of Reaction Ensemble Monte Carlo Algorithms to study the Kinetics of Polymerization"*, AIChE 2017 Conference , Minnesota, USA, 28 Oct - 3 Nov.
- 2017 Inderdip Shere and Ateeque Malani, Oral presentation: *"Understanding self-assembly of silica precursor using Monte Carlo simulation"*, CCP5, University of Strathclyde, UK, 21 - 23 May.
- 2016 Inderdip Shere and Ateeque Malani, Poster presentation: *"Studying Polymerization of Silica using Monte Carlo Simulation"*, 4th Soft Matter: Young Investigators Meet (SMYIM), The International Centre Goa (ICG), India, 16 - 18 Dec.
- 2016 Inderdip Shere and Ateeque Malani, Poster presentation: *"Study of Kinetics of Polymerization using Reaction Ensemble Monte Carlo"*, CheMference, Indian Institute of Technology Gandhinagar, Gujarat, India, 3 - 4 Dec.
- 2015 Inderdip Shere and Ateeque Malani, Poster presentation: *"Development of reaction algorithm of multi-functional precursor"*, Mumbai-Pune Soft Matter Meet, National Chemical Laboratory, Pune, India, 3 - 4 Dec.

Awards and Achievements

- 2017 **Best Three minute thesis talk:** *"Kinetic Study of Silica Polymerization Using Monte Carlo Simulation"*, Research Scholars' Symposium, Indian Institute of Technology Bombay, Mumbai, India.
- 2016 **Best Oral presentation:** *"Kinetics Studies of Silica Polymerization using Reaction Ensemble Monte Carlo"*, Research Scholars' Symposium, Indian Institute of Technology Bombay, Mumbai, India.
- 2015 **Best Poster presentation:** *"Monte Carlo Simulation of Silica Polymerization of Two, Three and Four Functional Alkoxides"*, Research Scholars' Symposium, Indian Institute of Technology Bombay, Mumbai, India.

Analytical and Computational Skills

Numerical methods & Statistical mechanics Monte Carlo technique (Reaction ensemble, capturing kinetics of MC move), Reaction kinetics and mechanism, Multi-scale modeling, Self-assembly, Forcefield development (PMF, Coarse-grain modeling), Molecular dynamics, Machine learning (DNN)

Technical Skills

Languages & Tools Fortran 90, C, OpenMP parallel computing, Matlab, Python, Bash script, Gromacs, Lammmps, Grace, VMD, Avogadro, Veusz, Latex, Quantum espresso

References

- Dr. Ateeque** (PhD advisor)
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- Dr. Jhumpa** (Research progress committee member)
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