SRITEJA MANTHA

Postdoctoral Research Associate, Chemistry and Chemical Engineering Division
California Institute of Technology, 1200 E Californa Blvd, Pasadena, CA-91125

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Education

University of Wisconsin-Madison, Madison-WI, USA
09/2011 —12/2016 || Ph.D. Chemistry
Advisor: Prof. Arun Yethiraj

Indian Institute of Technology, Kharagpur, India
08/2006 —05/2011 || Integrated Masters (5yr.) Industrial Chemistry
Institute Silver Medal

Research Experience

Postdoctoral Research:

California Institute of Technology, Pasadena-CA, USA
01/2020 —till date || *Advisor: Prof. Zhen-Gang Wang*

- Developed **enhanced sampling simulation** tools to design polyelectrolytes that prevent mineralization of calcium salts.
- Built novel **free energy perturbation** protocols to investigate the mechanism of **multivalent ion binding** to specific polymer residues.
- Built classical density functional theory and constructed **statistical analysis tools** such as transition path sampling to study nucleation in polymers.
- Explored synergetic combination of physics based molecular models and **machine learning tools** for materials discovery.
- Authored **two successful** research proposals that secured funding for Prof. Wang's research group.

Institute fur Physik, Universitat Mainz, Germany
01/2017 —12/2019 || *Advisor: Prof. Friederike Schmid*

- Developed **numerical models** such as self-consistent field theory and dynamic density functional theory to study self-assembly and dynamics of copolymers with **statistically distributed sizes**.

Graduate School Research:

University of Wisconsin-Madison, Madison-WI, USA
09/2011 —12/2016 || *Advisor: Prof. Arun Yethiraj*

- Constructed **molecular simulation** framework for **conformational analysis** of gemini surfactants that stabilize their self-assembly into bi-continuous network morphologies.
- Quantified **structure activity relationship** between the dynamics of nano-confined water and the chemical nature of the inerface, its curvature, hydration level of the confinement and the chemical nature of the counterion.

</> Skills

- Programming: C· Python · Matlab
- Machine Learning: Scikit-Learn · PyTorch

Coursera Certifications:

- Machine Learning Specialization
- Python Data Structures

Research Domain

- Chemical physics of surfactants
- Physics of polymer self-assembly & dynamics
- Computational modeling of rare events in chemical systems

Technical Skills

- Enhanced sampling molecular simulations
- Transition path sampling
- Self consistent field theory
- Classical density functional theory
- Dynamic density functional theory
- Statistical Associating fluid theory

Leadership, Mentoring and Service

- Co-organizer 2024 APS-DPOLY focus session on 'Machine Learning Assisted Polymer Design.'
- Co-mentor for the CCE division 2023 Caltech Rising-Tide program.
- Judge for the 2022 Caltech Undergraduate Summer Research Day.
- General Chemistry and Physical Chemistry Teaching Assistant, UW-Madison.
- Reviewer for the Journal of Physical Chemistry and Journal of Chemical Physics.

Publications

[13] S. Mantha, A. S. Ylitalo, H. Chao, V. Ginzburg, and Z.-G. Wang; Surfactant in a polyol-CO2 mixture: Insights from a classical density functional theory study, *Langmuir*, **38**, 16172 (2022)

[12] S. Mantha, S. Qi, and F. Schmid; Bottom-up construction of dynamic density functional theories for inhomogeneous polymer systems from microscopic simulations, *Macromolecules*, **53**, 3409 (2020)

[11] S. Mantha, S. Qi, M. Barz, and F. Schmid; How ill-defined constituents produce well-defined nanoparticles: Effect of polymer dispersity on the uniformity of copolymer micelles, *Physical Review Materials*, **3**, 026002 (2019)

[10] S. Mantha, G. Jackson, M. K. Mahanthappa, and A. Yethiraj; Counterion-regulated dynamics of water confined in lyotropic liquid crystalline morphologies, *Journal of Physical Chemistry B*, **122**, 2408 (2018)

[9] G. Jackson, S. Mantha, S.A. Kim, A. Yethiraj, and M. K. Mahanthappa; Ion specific confined water dynamics in convex nano pores of lyotorpic liquid crystals, *Journal of Physical Chemistry B*, **122**, 10031 (2018)

[8] S. Mantha, J. G. McDaniel, D. V. Perroni, M. K. Mahanthappa, and A. Yethiraj; Electrostatic interactions govern "Odd/Even" effects in water-induced gemini surfactant self-assembly, *Journal of Physical Chemistry B*, **121**, 565 (2017)

[7] J. G. McDaniel, S. Mantha, and A. Yethiraj; Dynamics of water in gemini surfactant based lyotorpic liquid crystals, *Journal of Physical Chemistry B*, **120**, 10860 (2016)

[6] S. Mantha, and A. Yethiraj; Dynamics of water confined in lyotorpic liquid crystals: Molecular dynamics simulations of the dynamic structure factor, *Journal of Chemical Physics*, **144**, 084504 (2016)

[5] S. Mantha and A. Yethiraj; Conformation properties of sodium polystyrene sulfonate in water: Insights from a. Coarse-grained model with explicit solvent, *Journal of Physical Chemistry B*, **119**, 11010 (2015)

[4] K. Charaborty, S. Mantha, and S. Bandyopadhyay; Molecular dynamics simulation of a single-stranded DN with heterogeneous distribution of nucleobases in aqueous medium, *Journal of Chemical Physics*, **139**, 075103 (2013)

Publications in Progress

[3] S. Mantha, A. Glisman, and Z.-G. Wang; Divalent ion mediated association between polyelectrolyte chains *(In preparation)*

[2] A. Glisman, S. Mantha, and Z.-G. Wang; Adsorption isotherm and the mechanism of divalent ion binding to polyelectrolyte *(In preparation)*

[1] S. Mantha, A. Glisman, and Z.-G. Wang; The Hydrophobe effect: Enhancing the solubility of polyelectrolyte-divalent ion complex *(In preparation)*

Talks & Presentations

[1] S. Mantha et.al, Ca^{2+} binding to polyelectrolytes, American Physical Society Meeting, March 2023 (Talk)

[2] S. Mantha et.al, Bubble nucleation in a surfactant stabilized polyol-CO2 mixture, American Institute of Chemical Engineers Annual Meeting, November 2022 (Talk)

[3] S. Mantha et.al, Effect of silicone surfactant on the CO2 bubble nucleation in polyol, Caltech Chemistry and Chemical Engineering Seminar Day, September 2021 (Invited Talk)

[4] S. Mantha et.al, Effect of silicone surfactant on the CO2 bubble nucleation in polyol, American Physical Society Meeting, March 2022 and March 2021 (Talk)

[5] S. Mantha et.al, Systematic Development of the Dynamic Density Functional Theory for Inhomogeneous Polymer Systems, Polymer Physics Group Meeting, Lincoln, UK, Sept 2019 (Poster and Talk)

[6] S. Mantha et.al, Dynamic Density Functional Theory Models for Inhomogeneous Polymer Systems , IRTG Meeting-Mainz, Germany , July 2019 (Invited Talk)

[7] S. Mantha et.al, Increasing block-copolymer dispersity leads to more uniform micelles, Gordon conference in polymer physics, July 2018 (Talk)

[8] S. Mantha et.al, Effect of polymer dispersity on the size of spherical micelles in solution, American Physical Society Meeting, March 2018 (Talk)

[9] S. Mantha et.al, Self assembly of anionic gemini surfactant molecules and property sof confined water, University of Wisconsin Materials Research Science and Engineering Center, April-2015 (Invited Talk)

[10] S. Mantha et.al, Effect of alkyl spacer length on the phase behavior of gemini dicarbocylate surfactant, American Conference on Theoretical Chemistry, July-2014 (Poster)

[11] S. Mantha et.al, Computer simulations of polyelectrolyte solutions, Midwest Theoretical Chemistry Conference, May-2013 (Poster)

Awards and Recognitions

2020 *Macromolecules* article highlighted in Advances in Engineering Magazine

2019 *Phys.Rev.Materials* article selected as Physical Review Editors Suggestion

2018 APS New Investigator Travel Award

2013 Telluride Science Center Summer Research Fellowship

2013 Outstanding Chemistry Teaching Award, University of Wisconsin—Madison

2013 Honored Instructor Award, University of Wisconsin—Madison

2011 Hirschfelder Graduate Student Award, University of Wisconsin—Madison

2011 Institute Silver Medal, Indian Institute of Technology—Kharagpur

2011 Institute Proficiency Award, Indian Institute of Technology—Kharagpur

2010 Prof. J.C. Ghosh Memorial Award, Indian Institute of Technology—Kharagpur

2009 Undergraduate Summer Research Fellowship,Indian Academy of Sciences

References

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