YAXIN AN

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EDUCATION

Ph.D. Chemical Engineering, Virginia Tech, Virginia, USA   08/2016-12/2020
M.S. Chemical Engineering, Tianjin University, Tianjin, China   09/2010-06/2013
B.S. Chemical Engineering, Central South University, Changsha, China   09/2006-06/2010

EXPERIENCE

Assistant Professor   08/2022-present
Department of Chemical Engineering, Louisiana State University
Research Interests: Molecular design of functional polymers, biomolecules and nanoparticles by computational simulations and data-driven approaches for health, sustainable and energy applications.

Postdoctoral Scholar   04/2021-07/2022
Department of Chemical and Biological Engineering, Princeton University
Advisers: Dr. Michael A. Webb and Dr. William M. Jacobs
Research Focus: Investigating the liquid-liquid phase separation behavior and rheological properties of intrinsically disordered proteins by integrating coarse-grained (CG) modeling and machine learning.

Graduate Research Assistant   08/2016-12/2020
Department of Chemical Engineering, Virginia Tech
Adviser: Dr. Sanket A. Deshmukh
Dissertation: Transferable Coarse-Grained Models: From Hydrocarbons to Polymers and Backmapped by Machine Learning
Research Projects:

11. Wang, Y., **An, Y. (co- rst author)**, Shmidov, Y., Bitton, R., Deshmukh, S. A., Matson, J., A combined experimental and computational approach reveals how aromatic peptide amphiphiles self-assemble to form ion-conducting nanohelices, Mater. Chem. Front., 4 (10), 3022-3031, *2020* (IF=6.5)

10. Conway, O., **An, Y.**, Bejagam, K., Deshmukh, S. A., Development of Transferable Coarse-Grained Models of Amino Acids, Mol. Syst. Des. & Eng., 5 (3), 675-685, *2019* (IF=4.9)

9. Solorzano, I., Bejagam, K., **An, Y.**, Singh. S., Deshmukh, S. A., Solvation dynamics of N-substituted acrylamide polymers and its importance on the phase transition behavior, Soft Matter, 16 (6), 1582-1593, *2019* (IF=3.7)

8. **An, Y.**, Singh, S.; Bejagam, K. K., Deshmukh, S. A. Development of an Accurate Coarse-Grained Model of Poly(acrylic acid) in Explicit Solvents , Macromolecules, 52 (13), 4875-4887, *2019* (IF=6.0)

7. Singh, S.; Bejagam, K. K., **An, Y.**, Deshmukh, S. A. Machine-Learning Based Stacked Ensemble Model for Accurate Analysis of Molecular Dynamics Simulations, J. Phys. Chem. A, 123 (24), 5190-5198, *2019* (IF=2.8)

6. **An, Y.**, Bejagam, K. K., Deshmukh, S. A. Development of Transferable Nonbonded Interactions between Coarse-Grained Hydrocarbon and Water Models, J. Phys. Chem. B, 123 (4), 909-921, *2019* (IF=3.0)

5. Bejagam, K. K.; **An, Y.**, Singh, S, Deshmukh, S. A. Machine-Learning Enabled New Insights into the Coil-to-Globule Transition of Thermosensitive Polymers Using a Coarse-Grained Model, J. Phys. Chem. Lett., 9 (22), 6480-6488, *2018* (IF=6.5)

9. Bejagam K. K., *An, Y.*, Singh S., Deshmukh, S. A., Machine Learning Enabled Insights into the Phase-Transition of Thermosensitive Polymers, ACS, Orlando, FL, USA, 2019 (**Oral**)

8. *Joshi, S.*, Y., Bejagam, K. K., **An, Y.**, Deshmukh, S. A., Studying Shape-Dependence of Structural Conformations for Coarse-Grained Thermo-Sensitive Bottle-Brush Polymer Models, AIChE, Orlando, FL, USA, 2019 (**Poster**)

7. *Sose, A.*, Singh, S., **An, Y.**, Deshmukh, S. A., Metal Organic Frameworks As Cargos for the Delivery of an Anti-Cancer Drug, Curcumin, AIChE, Orlando, FL, USA, 2019 (**Poster**)

6. **An, Y.**, Singh, S., Bejagam,K. K., Deshmukh, S. Aag-492(Si3i(461(DAccralte-460(Aoarse-1(n-Grained)-2