

# YAXIN AN

Department of Chemical Engineering, Louisiana State University

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## EDUCATION

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**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

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**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:**

- Collaborated with experimentalists to study the mechanism of self-assembly of peptide amphiphiles by using MARTINI models.
- Developed accurate transferable CG models of a variety of molecules: water, hydrocarbons, amino acids and polymers by using particle swarm optimization
- Constructed machine learning models such as artificial neural network (ANN) and k nearest neighbor (kNN) to backmap CG models into all-atom/united-atom models.

**Master Student** 09/2010-06/2013

**Department of Chemical Engineering, Tianjin University, China**

Adviser: Dr. Pingli Li

**Thesis:** Preparation of hollow fiber poly(vinylidene fluoride) membranes by thermally induced phase separation.

## HONORS & AWARDS

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Hord Graduate Fellowship, Virginia Tech 2020  
Graduate Travel Award, Virginia Tech 2019  
Outstanding Student, Tianjin University 2011  
National Encouragement Scholarship, Central South University 2009

## PEER-REVIEWED PUBLICATIONS

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[Google Scholar](#)

12. **An, Y.**, Deshmukh, S. A., Machine-learning approaches for backmapping coarse-grained models to all-atom models, ChemComm, 56 (65) 9312-9315, **2020** (IF=6.2)

11. Wang, Y., **An, Y. (co-first 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)  
*Virginia Tech Daily: Machine-learning enables a previously-unseen look at polymers helpful in biomedical field, Virginia Tech Daily, 2018*
4. Bejagam, K. K., Singh, S.; **An, Y.**, Deshmukh, S. A. Machine-Learned Coarse-Grained Models, *J. Phys. Chem. Lett.*, 9 (16), 4667-4672, **2018** (IF=6.5)  
*Virginia Tech Daily: New machine learning framework could lead to breakthroughs in material design, Virginia Tech Daily, 2018*
3. **An, Y.**, Bejagam, K. K., Deshmukh, S. A. Development of New Transferable Coarse-Grained Models of Hydrocarbons, *J. Phys. Chem. B*, 122 (28), 7143-7153, **2018** (IF=3.0)
2. Bejagam, K. K.; Singh, S., **An, Y.**, Berry, C.; Deshmukh, S. A. PSO-Assisted Development of New Transferable Coarse-Grained Water Models, *J. Phys. Chem. B*, 122 (6), 1958-1971, **2018** (IF=3.0)
1. Lin, L, Geng, H., **An, Y.**, Li, P., Chang, H. Preparation and properties of PVDF hollow fiber membrane for desalination using air gap membrane distillation, *Desalination*, 367, 145-153, **2015** (IF=9.5)

## CONFERENCE PRESENTATION

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*presenters' names are italic*

12. **An, Y.** Engineering Biological Condensates via Coarse-Grained Modeling and Machine Learning, ACS Middle Atlantic Regional Meeting, Ewing, NJ, 2022 (**Oral**)
11. **An, Y.** Combining Multi-Scale Modeling and Machine Learning to Design New Polymers and Biomolecules, AIChE, Boston, MA, USA, 2021 (**Poster**)
10. **An, Y.**, and Deshmukh, S. A., Solvent-Induced Conformation Transition of Bottlebrush Copolymers By Coarse-Grained Molecular Dynamics Simulations, AIChE, Orlando, FL, USA, 2019 (**Oral**)

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. A., An Accurate Coarse-Grained Model of Poly(acrylic acid) with Explicit Solvent Models of DMF and Water, AIChE, Orlando, FL, USA, 2019 (**Poster**)
5. Conway, O., **An, Y.**, Bejagam, K. K., Deshmukh, S. A., Development of Transferable Coarse-Grained Models of Amino Acids, AIChE, Orlando, FL, USA, 2019 (**Poster**)
4. **An, Y.**, Singh, S., Bejagam, K. K., Deshmukh, S. A., Development of Coarse-Grained Polystyrene and Poly(acrylic acid) Models—From Monomers to Polymer, Material Research Society, Boston, PA, USA, 2018 (**Oral**)
3. **An, Y.**, Bejagam, K. K., Deshmukh, S. A., Solvent Induced Coil-to-Globule Conformation Change of a Single Poly(acrylic acid) Chain, Material Research Society, Boston, PA, USA, 2018 (**Poster**)
2. **An, Y.**, Bejagam, K. K., Deshmukh, S. A., New Coarse-Grained Models of Hydrocarbons, AIChE, Minneapolis, MN, USA, 2017 (**Oral**)
1. **An, Y.**, Bejagam, K. K., Singh, S., Deshmukh, S. A., Atomic-level Comparisons of LCST Transition in Thermo-Sensitive Polymers. AIChE, Minneapolis, MN, USA, 2017 (**Oral**)

## TEACHING & MENTORING

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### Teaching Assistant

- CHE2114: Mass and Energy Balances, Teaching Assistant, Fall 2016
- CHE3015: Process Measurement and Control, Teaching Assistant, Spring 2020
- CHE4024: Unit Operations and Scale-Up, Teaching Assistant, Summer 2020

### Mentoring

- Ph.D. students: Soumil Joshi, Abhishek Sose, Virginia Tech, 2018-2019
- Undergraduates: Preeya Achari, Gaurav Anand, Virginia Tech, 2016-2018

## PROFESSIONAL SERVICE

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**Journal reviewer:** Physical Chemistry Chemical Physics, Computational Materials Science, RSC Advance.

**Conference symposium assistant:** Symposium BM03 at Materials Research Society, 2018.