Yaxin An, Ph.D. candidate

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EDUCATION

Ph.D. candidate, Chemcal Engineering, Virginia Tech, USA. (Supervisor: Dr. Sanket A. Deshmukh)   (2016 -present)
  Title: *Development of Coarse-Grained Models for Molecular Dynamics Simulations of Polymers*

Master of Science, Chemcal Engineering, Tianjin University, China (Supervisor: Dr. Pingli Li)   (2010 - 2013)
  Title: *Preparation of PVDF Hollow Fiber Membranes by the TIPS method*

Bachelor of Science, Chemical Engineering and Technology, Central South University, China   (2006 - 2010)

RESEARCH INTERESTS

Molecular Dynamics Simulations, Machine Learning, Optimization of Coarse-Grained Force-Fields, Polymers

RESEARCH EXPERIENCE

- **Research Assistanship**, Virginia Tech, USA.

  - Developed coarse-grained (CG) force-fields in molecular dynamics (MD) simulations by the Particle Swarm Optimization (PSO). Imporoved the convergency of PSO by aritificial neural network (ANN)

  - Employed data analytics to explore the relationship between CG force-fields parameters and properties of CG models.

  - Developed transferable CG models for hydrocarbons and optimized the interactions between CG hydrocarbon and water models.

  - Performed Gibbs free energy simulations by adaptive biased force method.

  - Developed the CG models of polymers in explicit solvent models to study its conformation transition induced by solvents.

  - Performed simulations of the self-assembly of block copolymers of polystyrene-poly(acrylic acid) in water/DMF solvent mixtures.

  - Investigated the conformations of bottlebrush copolymers with different architectures in different solvents by CG MD simulations.

  - Studied the self-assembly of peptide amphiphile using MARTINI models at timescale of tens of microseconds.

- **Master studernt**, Tianjin University, China. (Supervisor: Dr. Pingli Li)   (2010 - 2013)

  - Prepared hollow fiber polyvinylidene fluoride (PVDF) membranes via thermally induced phase separation (TIPS).

COURSE PROJECTS

- **Data Exploration and Prediction of Google Play Store Apps**, CS 5526, Data Analytics II, Virginia Tech, USA.

  - Analyzed the distribution of the positve, negative and neutral reviews made by users on the Google Play Store Apps.

  - Employed the natural language preprocessing toolkit in python to convert the reviews into bags of words and further to matrices for predictions.

  - Built the random forest classifier, logistic regression model, and XGB classifier to classify the reviews with different sentiments: positive, negative and neutral. The accuracy was around 87% for all of these models.

  - Developed the random forest classifier to classify the categories of apps based on their reviews. The accuracy, precision, recalls and F1 scores of the models were calculated.

- **Prediction of the Outcome of Dota 2 Matches**, CS 5824, Advanced Machine Learning, Virginia Tech, USA.

  - Two datasets were used for training the ANN model. One contains the games by all-level player, the other consisted of games by only top players.

  - Built the Artifical Neutral Network (ANN) to predict the game result of Dota 2 with different hero combinations.

  - The accuracy of the ANN models trained on the former and latter dataset reached ∼60% and ∼87%, respectively.

- **Movie Recommender System**, CS 5526, Data Analytic II, Virginia Tech, USA.

  - Analyzed the the MovieLens database to get the distribution of the number of rated movies by each user, and the distribution of the number of ratings receieved by each movie.

  - Built the movie recommender by user-user and item-item collaborative filtering techniques from scratch.

- **Optimization of the Ultrafiltration Process by Genetic Algorithm**, BSE 5046, Engineering Mathematics, Virginia Tech, USA.

  - The operation parameters in ultrafiltration processes were optimized to achieve high product selectivity and purity by genetic algorithm.

Awards/Fellowships

2019   **Graduate Travel Fund Award**, *Virginia Tech.*

2019   **2 million computing core hours**, *National Energy Research Scientific Computing Center (NERSC).*

Publications

- **An, Y.**, Signgh, S.; Bejagam, K. K., **An, Y.**, Deshmukh S. A. Development of an Accurate Coarse-Grained Model of Poly(acrylic acid) in Explicit Solvents , *Macromolecules*, **2019**, accepted.
- Signgh, S.; Bejagam, K. K., **An, Y.**, Deshmukh S. A. Machine-Learning Based Stached Ensemble Model for Accurate Analysis of Molecular Dynamics Simulations, *J. Phys. Chem. A*, **2019**, in press.
- **An, Y.**, Bejagam, K. K., Deshmukh S. A. Development of Transferable Nonbonded Interactions between Coarse-Grained Hydrocarbon and Water Models, *J. Phys. Chem. B*, **2019**, 4, 909-921.
- 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.*, **2018**, 9, 6480-6488.
- Bejagam, K. K., Singh, S.; **An, Y.**, Deshmukh S. A. Machine-Learned Coarse-Grained Models, *J. Phys. Chem. Lett.*, **2018**, 9, 4667-4672.
- **An, Y.**, Bejagam, K. K., Deshmukh S. A. Development of New Transferable Coarse-Grained Models of Hydrocarbons, *J. Phys. Chem. B*, **2018**, 122, 7143-7153.
- 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*, **2018**, 122, 1958-1971.
- 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*, **2015**, 367, 145-153.

Research Skills

Simulations: NAMD, LAMMPS, RASPA(basic)

Programming: Python, FORTRAN90, Matlab, bash scripting, awk, sed

Visualization: Matplotlib, Xmgrace

Press

2018   **Virginia Tech Daily** "New machine learning framework could lead to breakthroughs in material design"

2018   **Virginia Tech Daily** "Machine-learning enables a previously-unseen look at polymers helpful in biomedical field"

Teaching Experience

- Teaching assistant of the undergraduate course 'Mass Transfer and Balance'.   [Fall 2016]

Selected Presentations

2019   ACS National Meeting & Expo, Orlando, FL, USA

2018   Material Research Society, Boston, PA, USA

2017   AIChE Annual meeting, Minneapolis, MN, USA