Feng Gao

gaofeng2@msu.edu
Phone: 517-575-5686
3850 Coleman Rd, East Lansing, MI

EDUCATION

- **Ph.D., School of Computational Math, Science, and Engineering, 3.6/4.0** Sep 2016 – Jun 2019 (expected)
  Michigan State University, East Lansing, MI
- **Ph.D., Department of Plant, Soil and Microbial Sciences (computational toxicology), 3.6/4.0** Sep 2014 – Jun 2019 (expected)
  Michigan State University, East Lansing, MI
- **B.S., School of Chemistry and Chemical Engineering, 85/100** Sep 2010 – Jun 2014
  Nanjing University, Nanjing

HIGHLIGHTED SKILLS

- Machine learning, Data Mining, Natural Language Processing, mySQL, scikit-learn
- Data Structures, Algorithms, Python, C programming, R programming, Matlab, OpenMP, MPI, Tensorflow, Pytorch, Spark

RESEARCH EXPERIENCES

- **Research Assistant**, Michigan State University, East Lansing, MI Sep 2014 – present

  Wavelet scattering neural network for toxicity prediction of organic molecules
  - Wavelet scattering method on molecular graph for molecule feature generation
  - Sequence-to-sequence model for accuracy improvement
  - Achieved 87% accuracy with 10-fold cross validation using Tensorflow

  Message passing neural networks for chromatography retention time prediction
  - Gaussian representation of molecular electron density on mesh grids
  - Visualization of sub-structures learnt by neural network hidden layers
  - Achieved MAE 0.1 min in the leave-one-out cross validation using Tensorflow
- **Research Assistant**, Nanjing University, Nanjing Jan 2013 – Jun 2014

  Monte Carlo simulation of sequence length effects on crystallization of polymers
  - Home-made Monte Carlo simulation programs
  - Parallelization of programs using OpenMP

RELEVANT COURSEWORK

- Parallel Computing, Data Mining
- Math Foundation for Data Science, Numerical Linear Algebra, Statistical Methods

SELECTED PROJECTS

- **Parallel computing and profiling for molecular dynamics simulations: an MPI approach**

  - Keywords: Message Passing Interface(MPI); Parallel Computing; Profiling
  - Comparison of atom decomposition and spatial decomposition methods for MPI
  - MPI communications analysis with Multi Process Environment and visualization with jumpshot

- **Predictive Models for Acute Oral Systemic Toxicity (National Toxicology Program)**

  - Keywords: Data augmentation; Multitask learning; Substructure visualization

  - Visualization of neural network hidden layers to detect toxophore of pharmaceuticals
  - Multitask learning for accuracy improvement: 81% sensitivity and 80% specificity

Publications

- Wavelet scattering neural network for toxicity prediction of organic molecules, **Feng Gao,** Stephen A. Boyd, Brian Teppen, in preparation
- Message passing neural networks for chromatography retention time prediction, **Feng Gao,** Stephen A. Boyd, Brian Teppen, in preparation
- Mechanism Associated with Kaolinite Intercalation with Urea: Combination of Infrared Spectroscopy and Molecular Dynamics Simulation Studies, Shuai Zhang, Qinfu Liu, **Feng Gao**, Xiaoguang Li, Cun Liu, Hui Li, Stephen A. Boyd, Cliff T. Johnston, and Brian J. Teppen, J. *Phys. Chem. C*, 2017
- Thermodynamic Mechanism and Interfacial Structure of Kaolinite Intercalation and Surface Modification by Alkane Surfactants with Neutral and Ionic Head Groups, Shuai Zhang, Qinfu Liu, Hongfei Cheng, **Feng Gao**, Cun Liu, and Brian J. Teppen, *J. Phys. Chem. C, 2017*