Tianyu Gao

Carnegie Mellon University
515 S Aiken Ave, Apt 419, PA 15232
Email: gaotianyug94@gmail.com Tel: 412-954-8158

Education

Carnegie Mellon University Pittsburgh, PA Dec. 2016
- M.S. in Chemical Engineering
- **Overall GPA: 3.97/4, Major GPA: 4/4**
- Selected Courses: Analysis and Modeling of Transport Phenomenon, Process Systems Modeling, Mathematical Modeling of Chemical Engineering Processes, Molecular Simulation

Dalian University of Technology Dalian, China Jul. 2015
- B.S. with hornor in Chemical Engineering and Technology
- **Overall GPA: 90.84/100, Major GPA: 91.80/100**
- Selected Courses: Thermodynamics, Unit Operation, Chemical Reaction Engineering

Research & Industrial Experience

Graduate Thesis Carnegie Mellon University, PA Jan. 2016–
—Study of machine learned atomic metal potential energy surface Present
- Implemented density functional theory (DFT) and nudged elastic band (NEB) calculations using Vienna *Ab initio* Simulation Package (VASP).
- Applied a neural networks (NN) method to model Pd potential energies surface and performed large time scale molecular dynamics (MD) simulations for diffusion barrier estimation.
- Achieved an excellent accuracy of modeling ground and transit state potential energies and energy barriers at a speed several order faster than DFT calculations.

Undergraduate Thesis State Key Laboratory of Fine Chemicals, China Sept. 2014–
—Study on coated bimetallic nanocatalyst preparation and application May 2015
- Prepared silica coated CuNi bimetallic nanoparticles from reverse microemulsion by modified co-reduction method and characterized particles composition, size and morphology.
- Investigated catalysis activities of various compositions and sizes for *p*-nitrophenol reduction.
- Enhanced catalytic activity and selectivity compared to monometallic particles and studied bimetal synergetic effects.

Research Assistant State Key Laboratory of Fine Chemicals, China Apr. 2013–
—Highly enhanced photocatalytic activity of $Ag/AgCl/TiO_2$ by CuO co-catalyst May 2014
- Synthesized TiO_2 coated Cu/Ag/AgCl nanoparticles in a reverse microemulsion system.
- Evaluated photocatalytic activity by degradation of methyl orange and phenol under visible light.
- Improved photocatalytic efficiency significantly and studied mechanism through band gap theory and surface plasma resonance.

Intern, Group Leader Shenyang Research Institute of Chemical Industry, China June 2014–
- Simulated and optimized propylene-propane distillation process and designed affiliated facilities. July 2014
- Experimented in a diazols dye synthesis and studied the process of industrialized scale up.

Skills

Lab techniques: Gas chromatography-mass spectrometry (GC-MS), high performance liquid chromatography (HPLC), ultraviolet-visible spectroscopy (UV-vis), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD)

Software: VASP, Aspen Plus, Aspen Customer Model, GAMS, COMSOL Multiphysics, Simulink, Microsoft Office, ChemOffice, Origin

Programming Language: Python, Matlab, C, LaTeX

Publications

Yuzhen Ge, **Tianyu Gao**, *et al*, "Highly Efficient Silica Coated CuNi Bimetallic Nanocatalyst from Reverse Microemulsion," *Journal of Colloid and Interface Science*, 491 (2017): 123-132.

Tianyu Gao, John Kitchin, "Modeling Palladium surfaces with Density Functional Theory and Neural Networks," *Surface Science*, submitted.