

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 honor 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/TiO₂ by CuO co-catalyst

May 2014

- + Synthesized TiO₂ 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.
- + 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**, Cui Wang, Rongwen Lu, "Highly Efficient Silica Coated CuNi Bimetallic Nanocatalyst from Reverse Microemulsion," *Journal of Colloid and Interface Science*, accepted.

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