

## EDUCATION

### Carnegie Mellon University

Pittsburgh, PA

Dec. 2016

- + Master of Science in Chemical Engineering
- + **Overall GPA: 3.95/4, 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/TiO<sub>2</sub> by CuO co-catalyst

May 2014

- + Synthesized TiO<sub>2</sub> 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*, under third review.

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