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

- + Bachelor of Science in Chemical Engineering and Technology
- + Overall GPA: 90.4/100, Major GPA: 91.1/100
- + 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 high dimensional neural networks (NN) method to model Pd potential energies surface and performed large time scale molecular dynamics (MD) simulations.
- + Achieved an excellent accuracy of modeling ground and transit state potential energies at a speed several order faster than DFT calculations.

Course Project

Carnegie Mellon University, PA

Mar. 2016-

-Optimization of profit for Aspirin manufacture process

May 2016

- + Simulated Aspirin manufacture process in ASPEN and optimized profit using GAMS.
- + Implemented a PID controller on the crystallizer to stabilize reactor temperature.

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 coreduction 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.

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, LTEX

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, In Press.

Tianyu Gao, John Kitchin, "Neural Network, a Machine Learned Method for Metal Potential Energy surface," expected submition by the end of Oct.