Carnegie Mellon University 515 S Aiken Ave, Apt 419, PA 15232

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EDUCATION

Sept. 2015- Carnegie Mellon University

Pittsburgh, PA

Present

- Master of Science in Chemical Engineering
- **Service** 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

Sept. 2011-

Dalian University of Technology

Dalian, China

Jul. 2015

- Bachelor of Science in Chemical Engineering and Technology
- **S** Overall GPA: 90.4/100, Major GPA: 91.1/100
- Selected Courses: thermodynamics, unit operation, chemical reaction engineering

RESEARCH & INDUSTRIAL EXPERIENCE

Jan. 2016– Graduate Thesis

Carnegie Mellon University, PA

Present

- —Study of machine learned atomic metal potential energy surface
- 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.

Mar. 2016-

Course Project

Carnegie Mellon University, PA

May 2016

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

Sept. 2014-

Undergraduate Thesis

State Key Laboratory of Fine Chemicals, China

May 2015

- —Study on coated bimetallic nanocatalyst preparation and application
- 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.
- S Enhanced catalytic activity and selectivity compared to monometallic particles and studied bimetal synergetic effects.

Apr. 2013-

Research Assistant

State Key Laboratory of Fine Chemicals, China

May 2014

- —Highly enhanced photocatalytic activity of Ag/AgCl/TiO₂ by CuO co-catalyst
- ₩ Synthesized TiO₂ coated Cu/Ag/AgCl nanoparticles in a reverse microemulsion system.
- Figure 2 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.

June 2014-

Intern, Group Leader

Shenyang Research Institute of Chemical Industry, China

July 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, 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 submitting by the end of Oct.