Tianyu Gao

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Education

Sept. 2015– Present — **Carnegie Mellon University** — Pittsburgh, PA
- 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

Sept. 2011– Jul. 2015 — **Dalian University of Technology** — Dalian, China
- 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

Jan. 2016– Present — **Graduate Thesis** — Carnegie Mellon University, PA

—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.

Sept. 2014– May 2015 — **Undergraduate Thesis** — State Key Laboratory of Fine Chemicals, China

—Study on coated bimetallic nanocatalyst preparation and application
- 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.

Apr. 2013– May 2014 — **Research Assistant** — State Key Laboratory of Fine Chemicals, China

—Highly enhanced photocatalytic activity of $Ag/AgCl/TiO_2$ by CuO co-catalyst
- 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.

June 2014– July 2014 — **Intern, Group Leader** — Shenyang Research Institute of Chemical Industry, China
- 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, In Press
- **Tianyu Gao**, John Kitchin, "Neural Network, a machine learned method for Metal Potential Energy surface", Under Review