TIANYU GAO

Carnegie Mellon University
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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.

Mar. 2016–May 2016	**Course Project**	Carnegie Mellon University, PA

—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–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", expected submition by the end of Oct.