# Tianyu Gao

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## 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 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 $Ag/AgCl/TiO_2$ by CuO co-catalyst May 2014
- 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.

**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, LaTeX

## Publications

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