

## EDUCATION

<b>Carnegie Mellon University</b>	Pittsburgh, PA	Dec. 2016
<ul style="list-style-type: none"> <li>+ Master of Science in Chemical Engineering</li> <li>+ <b>Overall GPA: 3.95/4, Major GPA: 4/4</b></li> <li>+ Selected Courses: Analysis and Modeling of Transport Phenomenon, Process Systems Modeling, Mathematical Modeling of Chemical Engineering Processes, Molecular Simulation</li> </ul>		
<b>Dalian University of Technology</b>	Dalian, China	Jul. 2015
<ul style="list-style-type: none"> <li>+ Bachelor of Science in Chemical Engineering and Technology</li> <li>+ <b>Overall GPA: 90.84/100, Major GPA: 91.80/100</b></li> <li>+ Selected Courses: Thermodynamics, Unit Operation, Chemical Reaction Engineering</li> </ul>		

## RESEARCH & INDUSTRIAL EXPERIENCE

<b>Graduate Thesis</b>	Carnegie Mellon University, PA	Jan. 2016– Present
—Study of machine learned atomic metal potential energy surface <ul style="list-style-type: none"> <li>+ Implemented density functional theory (DFT) and nudged elastic band (NEB) calculations using Vienna <i>Ab initio</i> Simulation Package (VASP).</li> <li>+ Applied a high dimensional neural networks (NN) method to model Pd potential energies surface and performed large time scale molecular dynamics (MD) simulations.</li> <li>+ Achieved an excellent accuracy of modeling ground and transit state potential energies at a speed several order faster than DFT calculations.</li> </ul>		
<b>Undergraduate Thesis</b>	State Key Laboratory of Fine Chemicals, China	Sept. 2014– May 2015
—Study on coated bimetallic nanocatalyst preparation and application <ul style="list-style-type: none"> <li>+ Prepared silica coated CuNi bimetallic nanoparticles from reverse microemulsion by modified co-reduction method and characterized particles composition, size and morphology.</li> <li>+ Investigated catalysis activities of various compositions and sizes for <i>p</i>-nitrophenol reduction.</li> <li>+ Enhanced catalytic activity and selectivity compared to monometallic particles and studied bimetal synergetic effects.</li> </ul>		
<b>Research Assistant</b>	State Key Laboratory of Fine Chemicals, China	Apr. 2013– May 2014
—Highly enhanced photocatalytic activity of Ag/AgCl/TiO <sub>2</sub> by CuO co-catalyst <ul style="list-style-type: none"> <li>+ Synthesized TiO<sub>2</sub> coated Cu/Ag/AgCl nanoparticles in a reverse microemulsion system.</li> <li>+ Evaluated photocatalytic activity by degradation of methyl orange and phenol under visible light.</li> <li>+ Improved photocatalytic efficiency significantly and studied mechanism through band gap theory and surface plasma resonance.</li> </ul>		
<b>Intern, Group Leader</b>	Shenyang Research Institute of Chemical Industry, China	June 2014– July 2014
<ul style="list-style-type: none"> <li>+ Simulated and optimized propylene-propane distillation process and designed affiliated facilities.</li> <li>+ Experimented in a diazols dye synthesis and studied the process of industrialized scale up.</li> </ul>		

## 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, L<sup>A</sup>T<sub>E</sub>X

## 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*, under third review.

**Tianyu Gao**, John Kitchin, "Modeling Palladium surfaces with Density Functional Theory and Neural Networks," expected submission to *Surface Science* by the end of Dec.