Tianyu Gao

Carnegie Mellon University
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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

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, "Modeling Palladium surfaces with Density Functional Theory and Neural Networks," expected submition by the end of Oct.