Hanyu Ma

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RESEARCH INTERESTS

Computational models: Machine learning, first-principles and microkinetic simulations.

Advanced materials: Synthesis and characterization of structure-controlled nanomaterials.

Plasma catalysis: Renewable energy-based chemical transformations.

Environmental catalysis: Energy-efficient water treatment and air pollution control.

EDUCATION

Georgia Institute of Technology, Atlanta, GA, USA — Jan 2020 – present
- Online M.S. in Machine Learning — GPA: 4.00/4.00

University of Notre Dame, Notre Dame, IN, USA — Aug 2012 – May 2017
- Ph.D. in Environmental Engineering — GPA: 3.95/4.00

University of Notre Dame, Notre Dame, IN, USA — Aug 2014 – May 2016
- M.S. in Chemical Engineering — GPA: 4.00/4.00

Peking University, Beijing, CHN — Sep 2008 – Jul 2012
- B.E. in Environmental Engineering — Ranking: 3/22

HONORS AND AWARDS

Chinese Government Award for Outstanding Self-Financed Students Abroad, 2018
China Scholarship Council (1:200 award rate)
Notebaert Professional Development Award, University of Notre Dame 2017
The Patrick and Jana Eilers Graduate Student Fellowship, 2017
Notre Dame Energy (4 awardees per year)
Best Reviewer Award, *Journal of Environmental Sciences* (10 awardees per year) 2016
Conference Presentation Grant, University of Notre Dame 2013, 2016
SNO Student Award, Sustainable Nanotechnology Organization (10 awardees per year) 2016
Environmental Chemistry Graduate Student Award, 2016
American Chemical Society (20 awardees per year)
Bayer Predoctoral Research Fellowship, University of Notre Dame (2 awardees per year) 2014
Certificate of Merit Award (for presentation), 2013
246th American Chemical Society Meeting (15 awardees)
Innovative Undergraduates Fellowship, Peking University (5 awardees per year) 2011
President's Undergraduate Research Fellowship, Peking University 2010
May 4th Scholarship, Peking University (1:30 award rate) 2010
National Merit Scholarship, Peking University (1:50 award rate) 2009, 2010
1987 Alumni Scholarship, Peking University (1:30 award rate) 2009
Dean's award for Academic Excellence, Peking University (1:15 award rate) 2009

PROFESSIONAL

Postdoctoral Research Associate, University of Notre Dame, USA Jun 2017 – Present

- Advisor: William Schneider (Department Chair and Executive Editor of *J. Phys. Chem. C*)
- Department of Chemical and Biomolecular Engineering
  - Developed improved DFT and microkinetic models for catalytic water treatment by incorporating water as H-shuttle and solvent.
  - Developed models to elucidate the mechanism of plasma-enabled N_2 oxidation and predicted optimum catalysts with significantly enhanced activity.
  - Elucidated the structure-, temperature- and metal-dependent mechanisms for NH_3 oxidation using density functional theory and microkinetic modeling.

Research and Teaching Assistant, University of Notre Dame, USA Aug 2012 – May 2017

- Advisor: Chongzheng Na
- Department of Civil and Environmental Engineering and Earth Sciences
  - Developed robust nanocatalysts for advanced water treatment.
  - Elucidated size-controlled activation of Ru-catalyzed hydrogen release from NH_3BH_3.
  - Synthesized carbon-based nanomaterials for advanced water treatment.

PROFESSIONAL SKILLS

- **Computational modeling**: Vienna Ab Initio Simulation Package (VASP), microkinetic modeling, Gaussian, VASPsol and Atomic Simulation Environment.
- **Machine learning and data analysis via Python**: Pandas, SciPy, Scikit-learn, XGBoost, TensorFlow and Keras.
- **Programming languages**: Python, Matlab, SQL, Javascript, HTML and CSS.
- **Material synthesis**: Hydrothermal/solvothermal synthesis, chemical vapor deposition, microwave-assisted synthesis, incipient wetness impregnation and thermal phase transformation.
- **Material characterization**: Transmission electron microscopy, atomic force microscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, X-ray powder diffraction, single-crystal X-ray diffraction, X-ray fluorescence and BET surface area analysis.
- **Analytical chemistry**: Inductively coupled plasma-optical emission spectrometry and mass spectrometry, Fourier-transform infrared spectroscopy, high performance liquid chromatography, dynamic light scattering and UV-vis.

PUBLICATIONS

In Preparation

3. **H. Ma**, R. Sharma, S. Welzel, M. van de Sanden, W. Schneider and M. Tsampas, Enhancing potential of catalysts for plasma nitrogen oxidation, *in preparation*.
2. P. Nematollahi, **H. Ma**, W. Schneider, E. Neyts, DFT and microkinetic comparison of Ru-doped N-embedded graphene and nanotube toward catalytic formic acid formation and decomposition, *in preparation.*
1. **H. Ma**, D. Rensel, J. Hicks, C. Na, Lock-and-key in palladium phosphide catalyzed hydrodesulfurization, *in preparation*.

Journal Papers

11. **H. Ma**, W. Schneider, DFT and microkinetic comparison of Pt, Pd and Rh-catalyzed ammonia oxidation, ***Journal of Catalysis***, (383)2020, 322-330. IF=7.888.
10. **H. Ma**, S. Li, H. Wang, and W. Schneider, Water-mediated reduction of aqueous N-nitrosodimethylamine on Pd, ***Environmental Science & Technology***, (53)2019, 7551-7563. IF=7.864.
9. **H. Ma**, and W. Schneider, Structure- and temperature-dependence of Pt-catalyzed ammonia oxidation rates and selectivities, ***ACS Catalysis***, (9)2019: 2407-2414. IF=12.350.
8. **H. Ma**, H. Wang, P. Burns, B. McNamara, E. Buck, and C. Na, Synthesis and preservation of graphene-supported uranium dioxide nanocrystals, ***Journal of Nuclear Materials***, 475(2016): 113-122. IF=2.485. Rank: 2/34.
7. **H. Ma**, H. Wang, T. Wu, and C. Na, Highly active layered double hydroxide-derived cobalt nano-catalysts for *p*-nitrophenol reduction, ***Applied Catalysis B: Environmental***, 180(2016): 471-479. IF=16.683.
6. **H. Ma**, and C. Na, Isokinetic temperature and size-controlled activation of ruthenium-catalyzed ammonia borane hydrolysis, ***ACS Catalysis***, 5(2015).1726-1735. IF=12.350.
5. **H. Ma**, H. Wang, T. Wu, and C. Na, Microwave-assisted optimization of platinum-nickel nanoalloys for catalytic water treatment, ***Applied Catalysis B: Environmental***, 163(2015): 198-204. IF=16.683. **Featured by *Nanowerk* and in cover of *Elsevier*'s catalysis journals brochure**.
4. H. Wang,* **H. Ma**,* W. Zhen, D. An, and C. Na, Multifunctional and recollectable carbon nanotube ponytails for water purification, ***ACS Applied Materials & Interfaces***, 6(2014): 9426-9434. IF=8.758. *These authors contributed equally. **Featured by *Nanowerk***.
3. L. Cai, M. Tong, **H. Ma**, and H. Kim, Cotransport of titanium dioxide and fullerene nanoparticles in saturated porous media, ***Environmental Science & Technology***, 47(2013): 5703-5710. IF=7.864.

2. **H. Ma**, Y. Li, and Y. Liu, Preparation of refuse-derived fuel using screening residues of municipal solid waste and its combustion characteristics, ***Environmental Engineering***, 4(2012): 96-100. IF=NA.
1. **H. Ma**, Y. Ho, and H. Fu, Solid waste related research in Science Citation Index Expanded, ***Archives of Environmental Science***, 5(2011): 89-100. IF=NA.

Patents

2. C. Na, **H. Ma**, and H. Wang, Methods of making and using layered cobalt nano-catalysts, U.S. Patent Application No. 15/202,313.
1. C. Na, H. Wang, and **H. Ma**, Carbon nanotube ponytails. U.S. Patent Application No. 14/709,173.

Book Chapter

1. **H. Ma**, Reduce, reuse and recycle solid waste. In: X. Tang. [Ed.] *Household Environment and Health*. Higher Education Press: 2010.

AWARDED FUNDINGS AND RESOURCES

4. **H. Ma** (PI), Notre Dame Energy, The Patrick and Jana Eilers Graduate Student Fellowship: Size effect on ruthenium nanoparticle-catalyzed hydrogen generation from hydrazine borane, **Total awarded: $8,100**, 2017-2018.
3. **H. Ma** (PI), Notre Dame Center for Environmental Science and Technology, Bayer Predoctoral Research Fellowship: Two-dimensional nickel nano-catalysts for water treatment, **Total awarded: $10,250**, 2014-2015.
2. **H. Ma** (PI), Peking University, President's Undergraduate Research Fellowship: Preparation of refuse-derived fuel using screening residues of municipal solid waste, **Total awarded: $3,000**, 2010-2011.
1. W. Schneider (PI) and **H. Ma** (Preparer), National Energy Research Scientific Computing Center: Efficient coverage-aware DFT models for catalytic reactions on high-index faceted metals, **Total awarded: 150,000 CPU core hours**, 2019-2021.

TEACHING EXPERIENCE

Guest Lecturer, University of Notre Dame

1. CBE40447: Computational Chemistry Fall 2019
   - Gave guest lectures on Python and microkinetic modeling for 20 students.

Teaching Assistant, University of Notre Dame

5. CE30300: Introduction to Environmental Engineering Fall 2014
   - Gave review lectures before exams and QA lectures after exams for 60 students.
4. CE20230 Engineering Programming (MATLAB) Spring 2014

- Designed in-class quizzes and graded homework for 30 students.

3. CE31300: Introduction to Environmental Engineering Labs Fall 2013
   - Designed two lab experiments using my on-going research on experimental nanotechnology for water treatment for 30 students.
2. CE30320: Water Chemistry and Treatment Spring 2013
   - Office hours each week. Graded homework for 10 students.
1. CE30300: Introduction to Environmental Engineering Fall 2012
   - Office hours each week. Graded homework for 60 students.

Research Mentor, University of Notre Dame

2. NSF CISTAR Young Scholar Summer Research Summer 2018
   - Mentored an African-American student from high school on computational modeling of new phosphide catalysts for dehydrogenation.
1. Notre Dame International Summer Undergraduate Research Experience Summer 2017
   - Mentored a Hispanic master student from Sweden on fundamentals of density functional theory.

PROFESSIONAL ACTIVITIES

Journal Reviewer

ACS Catalysis, Journal of Physical Chemistry, Chemical Engineering Journal, Journal of Hazardous Materials, Catalysis Today, Chemosphere, International Journal of Chemical Kinetics, Journal of Environmental Sciences, Applied Nanoscience, Frontiers of Environmental Science & Engineering, Water Science & Technology, Water Science & Technology: Water Supply, Journal of Environmental Health Science & Engineering

Professional Affiliation

Member of American Chemical Society	2013 – Present
Member of Sustainable Nanotechnology Organization	2016 – Present
Member of Chicago Catalysis Club	2017 – Present
Member of American Institute of Chemical Engineers	2018 – Present
Member of Michigan Catalysis Society	2018 – Present

Service

4. Judge of Presentation Award, Chinese Environmental Scholars Forum 2019
3. Judge of Certificate of Merit Award, American Chemical Society 2018
2. Organizer, Notre Dame Catalysis Supergroup Biweekly Meetings 2017–Present
1. Presenter, 2016 Northern Indiana Regional Science and Engineering Fair 2016

CONFERENCE PRESENTATIONS

20. **H. Ma**, Water-mediated catalytic reactions for hydrogen generation and contaminant removal, *Environmental Engineering Research Seminar*, Texas A&M University, College Station, TX. March 2020. **Invited presentation**. Cancelled because of COVID-19.
19. **H. Ma**, Water-mediated catalytic reactions for hydrogen generation and contaminant removal, *Environmental Engineering Research Seminar*, Temple University, Philadelphia, PA. March 2020. **Invited presentation**.
18. **H. Ma**, Structure- and temperature-dependent catalysis: NH_3BH_3 hydrolysis and NH_3 oxidation, *Chemical Engineering Research Seminar*, University of Utah, Salt Lake City, UT. March 2020. **Invited presentation**.
17. **H. Ma**, Water-mediated catalytic reactions for hydrogen generation and contaminant removal, *Environmental Engineering Research Seminar*, University of Maine, Orono, ME. February 2020. **Invited presentation**.
16. **H. Ma**, and W. Schneider, Selectivity in multiple guises: Microkinetic models of ammonia catalytic oxidation, *2019 AIChE Annual Meeting*, Orlando, FL. November 2019. Oral presentation.
15. **H. Ma**, Structure- and temperature-dependent catalysis: NH_3BH_3 hydrolysis and NH_3 oxidation, *2019 Tim Taylor Department of Chemical Engineering Seminar, Kansas State University*, Manhattan, KS. October 2019. **Invited presentation**.
14. **H. Ma**, and W. Schneider, Selectivity in multiple guises: Microkinetic models of ammonia catalytic oxidation, *2019 North American Catalysis Society Meeting*, Chicago, IL. June 2019. Oral presentation.
13. **H. Ma**, S. Li, H. Wang, and W. Schneider, Water-mediated reduction of aqueous *N*-nitrosodimethylamine on Pd, *2019 Chinese Environmental Scholars Forum*, Houston, TX. June 2019. Oral presentation.
12. **H. Ma**, S. Li, H. Wang, and W. Schneider, Water-mediated reduction of aqueous *N*-nitrosodimethylamine on Pd, *2019 AEESP Research and Education Conference*, Tempe, AZ. May 2019. Poster presentation.
11. **H. Ma**, and W. Schneider, Selectivity in multiple guises: Microkinetic models of ammonia catalytic oxidation, *40th Annual Michigan Catalysis Society Spring Symposium*, Dearborn, MI. May 2019. Oral presentation.
10. **H. Ma**, and W. Schneider, Structure- and temperature-dependence of Pt-catalyzed ammonia oxidation rates and selectivities, *2018 AIChE Annual Meeting*, Pittsburgh, PA. October 2018. Oral presentation.
9. **H. Ma**, and W. Schneider, Temperature-dependent active sites of Pt catalyzed ammonia oxidation, *256th ACS National Meeting & Exposition*, Boston, MA. August 2018. Oral presentation.

8. **H. Ma**, and W. Schneider, Understanding selectivity in ammonia oxidation: DFT and microkinetic modeling over Pt, Pd and Rh (111), *Chicago Catalysis Club 2018 Spring Symposium*, Chicago, IL. May 2018. Poster presentation.
7. **H. Ma**, and W. Schneider, Understanding selectivity in ammonia oxidation: DFT and microkinetic modeling over Pt, Pd and Rh (111), *39th Annual Michigan Catalysis Society Spring Symposium*, Midland, MI. April 2018. Poster presentation.
6. **H. Ma**, D. Rensel, J. Hicks, and C. Na, Catalytic hydrodesulfurization of refractory sulfur compounds by crystalline and amorphous palladium phosphides, *SUNCAT Summer Institute 2017*, Menlo Park, CA. August 2017. Poster presentation.
5. **H. Ma**, T. Wu, and C. Na, Highly active palladium nanoparticles for catalytic reduction of N-nitrosodimethylamine, *253th ACS National Meeting & Exposition*, San Francisco, CA. April 2017. Oral presentation.
4. **H. Ma**, and C. Na. Abnormal size effect of metal-catalyzed contaminant reduction: Why bigger nanoparticles perform better, *2016 Sustainable Nanotechnology Organization Conference*, Orlando, FL. November 2016. Oral presentation.
3. **H. Ma**, and C. Na. Ruthenium-catalyzed ammonia borane hydrolysis: a curious case of nano-catalysis, *Environmental Engineering & Earth Sciences Seminar*, University of Notre Dame, IN. April 2015. Oral presentation.
2. **H. Ma**, H. Wang, and C. Na. Microwave-assisted synthesis of graphene-supported Pt@PtNi bimetallic nanoparticles as catalyst for nitroaromatic reduction, *Borchardt Conference*, University of Michigan, MI. February 2014. Poster presentation.
1. **H. Ma**, H. Wang, and C. Na. Settling and sorption behaviors of colloidal carbon nanotube bundles, *246th ACS National Meeting & Exposition*, Indianapolis, IN. September 2013. Poster presentation.