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EDUCATION

- 2009~2015 University of Texas at Austin, Austin, USA
Doctor of Philosophy in Physical Chemistry
Advisor: Prof. Graeme Henkelman
- 2005~2009 University of Science and Technology of China (USTC), Hefei, China
Bachelor of Science in Chemical Physics
Advisor: Prof. Jinlong Yang

PROFESSIONAL APPOINTMENTS

- 08/2018~present **Assistant Professor, University of Connecticut, Storrs, CT**
Department of Chemical and Biomolecular Engineering
- 08/2016~08/2018 **Post-doc Researcher, University of Pennsylvania, Philadelphia, PA**
Department of Chemical and Biomolecular Engineering
Advisor: Prof. Aleksandra Vojvodic
- 07/2015~08/2016 **Post-doc Researcher, Stanford University, CA**
Department of Chemical Engineering
Advisor: Prof. Jens. K. Nørskov and Dr. Aleksandra Vojvodic

HONORS AND AWARDS

- 2013 Graduate Student Professional Development Awards, University of Texas at Austin
- 2008 China National Awards for Inspiration, USTC
- 2005-2007 USTC Outstanding Student Scholarship, USTC
- 2005-2008 Cyrus Tang Scholarship for Personal Development and Community Service, USTC

PUBLICATIONS

- 27 Lucci, F. R.; **Zhang, L.**; Thuening, T.; Uhlman, M. B.; Schilling, A. C.; Henkelman, G.; Sykes, E. C. H., The Effect of Single Pd Atoms on the Energetics of Recombinative O₂ Desorption from Au (111). *Surface Science*, **2018**, 677, 296–300.
- 26 Akbashev, A.R.; **Zhang, L.**; Chueh, W.C.; Vojvodic, A. “Activation of SrTiO₃ with Subsurface SrRuO₃ for Oxygen Evolution Reaction”, **2018**, *Energy Environ. Sci.* **2018**, 11, 1762-1769 (**co-first author**).
- 25 Shin, K.; **Zhang, L.**; An, H.; Ha, H.; Yoo, M.; Lee, H. M.; Henkelman, G.; Kim, H. Y. “Interface Engineering for A Rational Design of Poison-free Bimetallic CO Oxidation Catalysts”, *Nanoscale*, **2017**, 9, 5244-5253. (**co-first author**).
- 24 Corona, B.; Howard, M.; **Zhang, L.**; Henkelman, G. “Computational Screening of Core-Shell Nanoparticles for the Hydrogen Evolution and Oxygen Reduction Reactions”, *J. Chem. Phys.*, **2016**, 145, 244708.
- 23 Luo, L.; **Zhang, L.**; Duan, Z.; Lapp, A. S.; Henkelman, G.; Crooks R. M. “Efficient CO Oxidation Using Dendrimer-Encapsulated Pt Nanoparticles Activated with <2% Cu Surface Atoms”, *ACS Nano.*, **2016**, 10, 8760-8769.

- 22 Kunal, P.; Li, H.; Dewing, B. L.; **Zhang, L.**; Jarvis, K.; Henkelman, G.; Humphrey S. M. "Microwave-Assisted Synthesis of PdAu Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity", *ACS Catal.*, **2016**, 6, 4882-4893.
- 21 Xiao, P.; Duncan, J.; **Zhang, L.**; Henkelman, G. "Ridge-Based Bias Potentials to Accelerate Molecular Dynamics", *J. Chem. Phys.*, **2015**, 143, 244104.
- 20 Anderson, R. M.; **Zhang, L.**; Wu, D.; Brankovic, S. R.; Henkelman, G.; Crooks R. M. "A Theoretical and Experimental In-Situ Electrochemical Infrared Spectroscopy Study of Adsorbed CO on Pt Dendrimer-Encapsulated Nanoparticles", *J. Electrochem. Soc.*, **2015**, 163, H3061.
- 19 **Zhang, L.**; Chill, S.; Henkelman, G. "Distributed Replica Dynamics", *J. Chem. Phys.*, **2015**, 143, 174112.
- 18 Luo, L.; **Zhang, L.**; Henkelman, G.; Crooks R. M. "Unusual Activity Trend for CO Oxidation on PdAu_{nan}@Pt Core@shell Nanoparticle Electrocatalysts", *J. Phys. Chem. Lett.*, **2015**, 6, 2562-2568. (co-first author)
- 17 Yu, W.-Y.; **Zhang, L.**; Mullen, G.; Henkelman G.; Mullins, C. B. "Effect of Annealing in Oxygen on Alloy Structures of Pd-Au Bimetallic Model Catalysts", *Phys. Chem. Chem. Phys.*, **2015**, 17, 20588-20596.
- 16 Yu, W.-Y.; **Zhang, L.**; Mullen, G.; Henkelman G.; Mullins, C. B. "Oxygen Activation and Reaction on Pd-Au Bimetallic Surfaces", *J. Phys. Chem. C*, **2015**, 119, 11754-11762.
- 15 Anderson, R. M.; Yancey, D. F.; **Zhang, L.**; Chill, S. T.; Henkelman, G.; Crooks R. M. "A Theoretical and Experimental Approach for Correlating Nanoparticle Structure and Electrocatalytic Activity", *Acc. Chem. Res.*, **2015**, 48, 1351-1357.
- 14 **Zhang, L.**; Anderson, R. M.; Crooks R. M.; Henkelman, G. "Correlating Structure and Function of Metal Nanoparticles for Catalysis", *Surf. Sci.*, **2015**, 640, 65-72.
- 13 Mullen, G. M.; **Zhang, L.**; Evans, E. J. Jr; Yan, T.; Henkelman, G.; Mullins, C. B. "Control of Selectivity in Allylic Alcohol Oxidation on Gold Surfaces: The Role of Oxygen Adatoms and Hydroxyl Species", *Phys. Chem. Chem. Phys.*, **2015**, 17, 4730-4738.
- 12 **Zhang, L.**; Henkelman, G. "Computational Design of Alloy-Core@Shell Metal Nanoparticle Catalysts", *ACS Catal.*, **2015**, 5, 655-660.
- 11 Garcia, S.; **Zhang, L.**; Piburn, G. W.; Henkelman, G.; Humphrey, S. M. "Microwave Synthesis of Classically Immiscible Rhodium-Silver and Rhodium-Gold Alloy Nanoparticles: Highly Active Hydrogenation Catalysts", *ACS Nano*, **2014**, 8, 11512-11521.
- 10 Chill, S. T.; Welborn, M.; Terrell, R.; **Zhang, L.**; Berthet, J.-C.; Pedersen, A; Jónsson, H.; Henkelman, G. "EON: Software for Long Time Simulations of Atomic Scale Systems", *Model. Simul. Mater. Sci. Eng.*, **2014**, 22, 055002.
- 9 Mullen, G. M.; **Zhang, L.**; Evans, E. J. Jr; Yan, T.; Henkelman, G.; Mullins, C. B. "Oxygen and Hydroxyl Species Induce Multiple Reaction Pathways for the Partial Oxidation of Allyl Alcohol on Gold", *J. Am. Chem. Soc.*, **2014**, 136(17) 6489-6498.
- 8 Anderson, R. M.; **Zhang, L.**; Frenkel, A. I.; Henkelman, G.; Crooks R. M. "Structural Study of the Inversion of Pd@Pt Core@Shell Dendrimer-Encapsulated Nanoparticles and Comparison to Theory", *ACS Nano*, **2013**, 7, 9345-9353.
- 7 **Zhang, L.** and Henkelman, G. "Design of Pt-shell Nanoparticles with Alloy Cores for the Oxygen Reduction Reaction", *ACS Nano*, **2013**, 7, 9168-9172.
- 6 **Zhang, L.**; Kim, H. Y.; Henkelman, G. "CO Oxidation at the Au-Cu Interface of Bimetallic Nanoclusters Supported on CeO₂ (111)", *J. Phys. Chem. Lett.*, **2013**, 4, 2943-2947.
- 5 Yancey, D. F.; Chill, S. T.; **Zhang, L.**; Frenkel, A. I.; Henkelman, G.; Crooks, R. M. "A Theoretical and Experimental Examination of Systematic Ligand-Induced Disorder in Au Dendrimer Encapsulated Nanoparticles", *Chem. Sci.*, **2013**, 4, 2912-2921.
- 4 Iyyamperumal, R.; **Zhang, L.**; Henkelman, G.; Crooks, R. M. "Efficient Electrocatalytic Oxidation of Formic Acid Using Au@Pt Dendrimer Encapsulated Nanoparticles", *J. Am. Chem. Soc.*, **2013**, 135, 5521-5524.
- 3 **Zhang, L.**; Henkelman, G. "Tuning the Oxygen Reduction Activity of Pd Shell Nanoparticles with Random Alloy Cores", *J. Phys. Chem. C*, **2012**, 111, 120860-120865.
- 2 Yancey, D. F.; **Zhang, L.**; Crooks, R. M.; Henkelman, G. "Au@Pt Dendrimer Encapsulated Nanoparticles as Model Electrocatalysts for Comparison of Experiment and Theory", *Chem. Sci.*, **2012**, 4, 1033.
- 1 Tang, W.; **Zhang, L.**; Henkelman, G. "Catalytic Activity of Pd/Cu Random Alloy Nanoparticles for Oxygen Reduction", *J. Phys. Chem. Lett.*, **2011**, 11, 1328-1331.

CONFERENCE PRESENTATIONS

Talks:

- Nov 2017 **Zhang, L.;** Vojvodic, A. "Rational Design of Novel Core-shell Material for Energy Conversion", *2017 AIChE Annual Meeting*, Minneapolis, MN.
- Nov 2016 **Zhang, L.;** Henkelman, G. "Computational Design of Novel Core@shell Nanoparticles for Catalysis", *2016 AIChE Annual Meeting*, San Francisco, CA.
- Jun 2016 **Zhang, L.;** Vojvodic, A. "Under and Above the Cover: Towards Understanding the Role of the 2D Cover", *Institute for Pure and Applied Math (IPAM): Materials for a Sustainable Energy Future Reunion Conference*, Lake Arrowhead, CA.
- Oct 2013 Henkelman, G.; **Zhang, L.** "Modeling the Structure and Activity of Nanoparticle Catalysts", *IPAM: Materials for a Sustainable Energy Future*, Los Angeles, CA. (split-talk with Prof. Henkelman)
- Apr 2013 **Zhang, L.;** Henkelman, G. "Alloy-Core@Shell Nanoparticles for Oxygen Reduction Reaction(ORR)", *245th ACS National Meeting*, New Orleans, LA.

Posters:

- Nov 2016 **Zhang, L.;** Fredrickson, K. D.; Vojvodic, A. *2016 AIChE Annual Meeting*, San Francisco, CA.
- Aug 2015 **Zhang, L.;** Henkelman, G. *SUNCAT Summer School 2015: Heterogeneous Catalysis for Energy and Society*, Menlo Park, CA.
- Feb 2015 **Zhang, L.;** Henkelman, G. *Center for Electrochemistry (CEC) Annual Workshop on Electrochemistry*, Austin, TX.
- Jul 2014 **Zhang, L.;** Henkelman, G. *American Conference on Theoretical Chemistry (ACTC)*, Telluride, CO.
- Jun 2014 **Zhang, L.;** Henkelman, G. *Gordon Research Conference: Catalysis*, New London, NH.
- May 2013 **Zhang, L.;** Henkelman, G. *Freshman Research Initiative (FRI): 2013 Inaugural Annual Conference*, Austin, TX.
- Nov 2012 **Zhang, L.;** Henkelman, G. *2012 Materials Research Society(MRS) Fall Meeting*, Boston, MA.

REVIEW

Regularly review articles for *J. Phys. Chem C, Phys. Chem. Chem. Phys., J. Mater. Chem. A.*