

# Liang Zhang

## PERSONAL INFO

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## EDUCATION AND TRAINING

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**Post-doctoral Fellow** 08/15/2015 - present

*Supervisor: Prof. Jens. K. Nørskov*  
Stanford University, Stanford, USA

**Doctor of Philosophy** in Physical Chemistry 08/15/2009-8/15/2015

*Supervisor: Prof. Graeme Henkelman*  
The University of Texas at Austin, Austin, USA **GPA: 4.00**  
• *Graduate Student Professional Development Awards* (Apr 2013)

**Bachelor of Science** in Chemical Physics 07/01/2005-05/30/2009

*Supervisor: Prof. Jinlong Yang*  
The University of Science and Technology of China, Hefei, China **GPA: 3.82**  
• *National Awards for Inspiration* (2008)  
• *Outstanding Student Scholarship* (2005-2007)

## RESEARCH INTERESTS

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**Computation Aided Novel Catalysts Discovery** Optimization of catalytic properties of nanoparticles using *Ab initio* calculation. Search for general correlations between the structures and functions to collaborate with experiment groups for advanced catalysts design. High-throughput computation and screening of catalysts based on the structure-function correlation.

**Catalytic Processes on Surface:** First principal simulations of catalytic processes on surface and complex media, such as metal oxide supported nanoparticles. Engineering the metal-support interaction for rational design of functional catalysts. Collaborative

study with experiment group to identify transition states and reaction pathways. Applying micro-kinetic analysis to understand the correlation between reaction rate and descriptors.

**Long Timescale Dynamics using Accelerated MD** Algorithms development and modeling of chemical processes over long times for distributing computing system. Contributed to implementation and maintenance of the accelerated MD part of EON software package (a distributed simulation package written in C++ and Python).

## PUBLICATIONS

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1. **Zhang, L.**; Chill, S.; Henkelman, G. "Distributed Replica Dynamics", *J. Chem. Phys.*, **143**, 174112 (2015).
2. Luo, L.; **Zhang, L.**; Henkelman, G.; Crooks R. M. "Unusual activity trend for CO oxidation on Pd<sub>x</sub>Au<sub>140-x</sub>@Pt core@shell nanoparticle electrocatalysts", *J. Phys. Chem. Lett.*, **6**, 2562-2568 (2015).
3. Yu, W.-Y.; **Zhang, L.**, Mullen, G.; Henkelman G.; and Mullins, C. B. "Effect of annealing in oxygen on alloy structures of Pd-Au bimetallic model catalysts", *Phys. Chem. Chem. Phys.*, **17**, 20588-20596 (2015).
4. Yu, W.-Y.; **Zhang, L.**, Mullen, G.; Henkelman G.; and Mullins, C. B. "Oxygen Activation and Reaction on Pd-Au Bimetallic Surfaces", *J. Phys. Chem. C*, **119**, 11754-11762 (2015).
5. 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.* , **48**, 1351-1357 (2015).
6. **Zhang, L.**; Anderson, R. M; Crooks R. M; Henkelman, G. "Correlating Structure and Function of Metal Nanoparticles for Catalysis", *Surf. Sci.*, **640**, 65-72 (2015).
7. 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.*, **17**, 4730-4738 (2015).
8. **Zhang, L.**; Henkelman, G. "Computational design of alloy-core@shell metal nanoparticle catalysts", *ACS Catal.*, **5**, 655-660 (2015).
9. 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*, **8**, 11512-11521 (2014).

10. Chill, S. T.; Welborn, M.; Terrell, R.; **Zhang, L.**; Berthet, J-C.; Pedersen, A; Jonsson, H.; Henkelman, G. "EON: Software for Long Time Simulations of Atomic Scale Systems", *Model. Simul. Mater. Sci. Eng.* , **22**, 055002 (2014).
11. 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.*, **136(17)**, 6489-6498 (2014).
12. 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*, **7**, 9345-9353 (2013).
13. **Zhang, L.** and Henkelman, G. "Design of Pt-shell Nanoparticles with Alloy Cores for the Oxygen Reduction Reaction", *ACS Nano*, **7**, 9168-9172 (2013).
14. **Zhang, L.**; Kim, H. Y.; Henkelman, G. " CO Oxidation at the Au-Cu Interface of Bimetallic Nanoclusters Supported on CeO<sub>2</sub>(111)," , *J. Phys. Chem. Lett.* **4**, 2943-2947 (2013).
15. 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.* **4**, 2912-2921 (2013).
16. Iyyamperumal, R.; **Zhang, L.**; Henkelman, G.; Crooks, R. M. "Efficient Electro- catalytic Oxidation of Formic Acid using Au@Pt Dendrimer Encapsulated Nanoparticles", *J. Am. Chem. Soc.* **135**, 5521-5524 (2013).
17. **Zhang, L.**; Henkelman, G. "Tuning the Oxygen Reduction Activity of Pd Shell Nanoparticles with Random Alloy Cores", *J. Phys. Chem. C* **111**, 120860-120865 (2012).
18. 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.* **4**, 1033 (2012).
19. Tang, W.; **Zhang, L.**; Henkelman, G. "Catalytic Activity of Pd/Cu Random Alloy Nanoparticles for Oxygen Reduction", *J. Phys. Chem. Lett.* **11**, 1328-1331 (2011).

## CONFERENCES

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1. **Zhang, L.**; Howard, M.; Henkelman, G. *American Conference on Theoretical Chemistry (ACTC)* , Telluride , CO. **Jul 2014**
2. **Zhang, L.**;Howard, M.; Henkelman, G. *Gordon Research Conference: Catalysis* , New London, NH. **Jun 2014**

3. Henkelman, G. and **Zhang, L.** *Institute for Pure and Applied Math, Long Program: Materials for a Sustainable Energy Future Program Fuels from Sunlight* , Los Angeles, CA. **Oct 2013**
4. **Zhang, L.** and Henkelman, G. *SLAC/Stanford Summer School 2013: Heterogenous Catalysis for Energy Transformations* , Menlo Park, CA. **Aug 2013**
5. **Zhang, L.**; Stauffer, S.; Henkelman, G. *Freshman Research Initiative: 2013 Inaugural Annual Conference* , Austin, TX. **May 2013**
6. **Zhang, L.**; Iyyamperumal, R.; Crooks, R. M.; Henkelman, G. *245th ACS National Meeting* , New Orleans, LA. **Apr 2013**
7. **Zhang, L.**; Tang, W.; Henkelman, G. *2012 Materials Research Society Fall Meeting* , Boston, MA. **Nov 2012**
8. **Zhang, L.**; Yancey, D. F.; Crooks, R. M. and Henkelman, G. *Institute for Pure and Applied Math, Long Program: Navigating Chemical Compound Space for Materials and Bio Design* , Los Angeles, CA. **May 2011**