

Meng Zhao

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EDUCATION

Case Western Reserve University, Cleveland, Ohio

Doctor of Philosophy in Chemistry (GPA: 3.7/4.0)

Aug. 2011- May 2017

Thesis Topic: Understanding electrochemical interface properties by comprehensive self-consistent density functional theory

Advisor: Alfred B. Anderson

Northwest University, Xi'an, China

B.S. in Chemistry (GPA: 3.5/4.0)

Sep. 2007 - July 2011

HONORS AND AWARDS

- Graduate Dean's Instructional Excellence Award, Case Western Reserve University, **2017**
- Best Teaching Assistant Award, Chemistry Department of Case Western Reserve University, **2017**
- Electrochemical Society Travel Award, Electrochemical Society(ECS), **2016**
- School of Graduate Student Travel Award, Case Western Reserve University, **2015**

RESEARCH EXPERIENCE

Department of Chemical Engineering, Stanford University, Menlo Park, California

Postdoctoral Researcher, Advisor: Thomas Bligaard/Jens Norskov

June. 2017 – Present

Department of Chemistry, Case Western Reserve University, Cleveland, Ohio

Research Assistant, Advisor: Alfred B. Anderson

Aug. 2011 – May 2017

1. Development of simulation techniques and models to explain industrial catalytic behaviors for process improvements:

- Proposed an autocatalytic mechanism of electroless Cu deposition on Cu electrode in alkaline electrolytes by characterizing transition states, predicting potentials for surface reactions with linear Gibbs energy relationship (LGER) and analyzing electron distributions.
- Investigated the potential-dependent coverage of H(ads) and hydrogen evolution reactions(HER) on the Cu(111) surface.

2. Fundamental understandings of the relationship between electrolyte pH and the potentials for surface reactions:

- Calculated onset potentials for H(ads) and OH(ads) on Pt(111) at different pH with density functional theory (DFT) applying two-dimensional periodic boundary conditions.
- Developed a systematic procedure extracting onset potentials from cyclic voltammograms.

3. Utilize Haber cycles to correlate chemical and electrochemical properties:

- Provided a new electrochemical perspective predicting dissociation energies of adsorbates on Pt(111) surface from its electrode potentials.

4. Prepare supportive documentations for technical training:

- Wrote hands-on users' manuals for home-made computational codes.

SKILLS AND TECHNIQUES

- Programming and Computer Skills: Python
- Operating Systems: Unix/Linux, Windows, Mac OS
- Computational Chemistry and General Computational Tools: ASE, Quantum Espresso, Gaussian 09, VASP (Vienna Ab-initio Simulation Package), INTERFACE 1.0 (Density Functional Theory code)

- Other software packages: WinSCP, Cygwin, Origin 8.1, Mathematica, Crimson Editor SVN 286, Adobe Photoshop, Microsoft Office: Word, Excel, PowerPoint, Outlook
- Knowledge of quantum chemistry, physical chemistry, electrochemistry, transport processes, density functional theory, semi-empirical methods, first-principles computation of material properties, statistical mechanics concepts and have experiences with high-performance computer clusters (HPCC) environments

TEACHING AND LEADERSHIP EXPERIENCE

Senior Teaching Assistant Coordinator and Teaching Assistant

Sept. 2013 – May 2017

- Effectively managed a team of seven teaching assistants for successful TA assignment completion while monitoring for top productivity.
- Maintained effective communications with, and between, professors and teaching assistants to secure working efficiency.

Lab Instructor

Sept. 2012 – Sept. 2013

- Closely supervised twelve undergraduate students in organic chemistry laboratory while providing exceptional support and assistance to ensure optimal student success

PUBLICATIONS

1. **M. Zhao** and A. B. Anderson, "Theory of Hydrogen Deposition and Evolution on Cu(111) Electrodes." *J. Electrochem. Soc.* **2017**, *164(9)*, H691-H695.
2. **M. Zhao**, L. Yu, R. Akolkar, and A. B. Anderson, "Mechanism of Electroless Copper Deposition from $[\text{Cu}^{\text{II}}\text{EDTA}]^{2-}$ Complexes Using Aldehyde-based Reductants." *J. Phys. Chem. C* **2016**, *120 (43)*, 24789-24793.
3. **M. Zhao** and A. B. Anderson, "Predicting pH Dependencies of Electrode Surface Reactions in Electrocatalysis." *Electrochem. commun.*, **2016**, *69*, 64-67.
4. **M. Zhao** and A. B. Anderson, "Predicting Reaction Mechanisms and Potentials in Acid and Base from Self-Consistent Quantum Theory: H(ads) and OH(ads) Deposition on the Pt (111) Electrode." *J. Phys. Chem. Lett.*, **2016**, *7*, 711–714.
5. A. B. Anderson and **M. Zhao**, "Reaction Energy for an Electrode Surface Atom Inserting into an R-H Bond and Its Dependence on Electrode Potential: Application to Pt (111)." *J. Electrochem. Soc.* **2015**, *162(9)*, H583-H589.

PRESENTATIONS

1. Two Oral Presentations, 229th Electrochemical Society (ECS) Conference, San Diego, CA: 2016
2. Poster Presentation, 47th Central Regional Meeting of the American Chemical Society, Covington, KY: 2016
3. Poster Presentation, Energy Materials Nanotechnology (EMN) Meeting, Orlando, FL: 2016
4. Poster Presentation, 228th Electrochemical Society (ECS) Conference, Phoenix, AZ: 2015
5. Poster Presentation, Research ShowCASE, Case Western Reserve University, Cleveland, OH: 2014, 2015
6. Poster Presentation, Spring Meeting of the Pittsburgh-Cleveland Catalysis Society, Carnegie Mellon University, Pittsburgh, PA: 2014