

Zhixiao Liu
Ph. D candidate
Department of Mechanical Engineering
Texas A&M University
Tel.: 979-587-2388 E-mail: liuzhixiao1985@tamu.edu; liuzhixiao@gmail.com

EDUCATION

- **Texas A&M University**, College Station, Texas, United States
Ph. D, Department of Mechanical Engineering August 2012-present
Thesis: Mesoscale interactions in electrodes for energy storage
Advisor: Dr. Partha P. Mukherjee
- **Hunan University**, Changsha, Hunan, China September 2009-June 2012
M. S., Department of Applied Physics
Thesis: Adsorption and dissociation of oxygen-contained gas molecule on uranium surface: a first-principles study
Advisor: Dr. Huiqiu Deng
- **Hunan University**, Changsha, Hunan, China September 2005-June 2009
B. S., Department of Applied Physics
Thesis: First-principle study of CO adsorption on γ -uranium (001) surface
Advisor: Dr. Huiqiu Deng

RESEARCH EXPERIENCE

- Research Assistant**, Energy and Transport Sciences Lab, Texas A&M University June 2013-present
- Mesoscale modeling of processing influenced electrode microstructure evolution in Li-ion battery.
 - Developing a bottom-up mesoscale framework to investigate precipitation induced microstructure evolution in Li-S battery (funded by U. S. Department of Energy).
- Research Assistant**, Atomic Simulation Lab, Hunan University September 2009-June 2012
- Studying gas molecules adsorption on uranium surface (funded by National Science Foundation of China)
- Undergraduate Research**, Atomic Simulation Lab, Hunan University November 2008-June 2009
- Studying CO adsorption on uranium surface

TEACHING EXPERIENCE

- Undergraduate Student Mentor**, Texas A&M University May 2013-December 2013
- Dion Hubble, Chemical Engineering, topic: properties of Li_2S surface.
- Teaching Assistant**, Texas A&M University August 2012-May 2013
- MEEN 222, Material Science
- Teaching Assistant**, Hunan University September 2009-June 2011
- Solid State Physics for undergraduate

SOFTWARE EXPERIENCE

Computer Programing: C/C++; Matlab.
Atomistic Simulation: VASP; Quantum Espresso.

JOURNAL PUBLICATIONS

1. **Z. Liu**, P. Balbuena, P. P. Mukherjee, "Evaluating Silicene as a Potential Cathode Host to Immobilize Polysulfides in Lithium-Sulfur Batteries", *J. Coord. Chem.*, **in press** (2016)
2. **Z. Liu**, S. Bertolini, P. Balbuena, P. P. Mukherjee, "Li₂S Film Formation on Lithium Anode Surface of Li-S Batteries", *ACS Appl. Mater. Interfaces*, **8**, 4700 (2016)
3. A. D. Dysart, J. C. Burgos, A. Mistry, C.-F. Chen, **Z. Liu**, C. N. Hong, P. Balbuena, P. P. Mukherjee, V. Pol, "Towards Next Generation Lithium-Sulfur Batteries: Non-conventional Carbon Compartments/Sulfur Electrodes and Multi-scale Analysis", *J. Electrochem. Soc.*, **163**, A730 (2016)
4. **Z. Liu**, B. Deng, G. J. Cheng, H. Deng, P. P. Mukherjee, "Mesoscale Elucidation of Laser-Assisted Chemical Deposition of Sn Nanostructured Electrodes", *J. Appl. Phys.*, **117**, 214301 (2015)
5. **Z. Liu**, D. Hubble, P. B. Balbuena, P. P. Mukherjee, "Adsorption of Insoluble Polysulfides Li₂S_x (x = 1, 2) on Li₂S Surfaces", *Phys. Chem. Chem. Phys.*, **17**, 9032-9039 (2015)
6. **Z. Liu**, H. Deng, P. P. Mukherjee, "Evaluating Pristine and Modified SnS₂ as a Lithium-ion Battery Anode: a First-principles Study", *ACS Appl. Mater. Interfaces*, **7**, 4000-40009 (2015)
7. **Z. Liu**, H. Deng, Q. Su, J. Liu, W. Hu, "Stability and Diffusion Properties of Ti Atom on α -Uranium Surfaces: A First-Principles Study", *Comput. Mater. Sci.*, **97**, 201-208 ((2015)
8. **Z. Liu**, V. Battaglia, P. P. Mukherjee, "Mesoscale Elucidation of the Influence of Mixing Sequence in Electrode Processing", *Langmuir*, **30**, 15102-15113 (2014)
9. **Z. Liu**, P. P. Mukherjee, "Microstructure Evolution in Lithium-Ion Battery Electrode Processing, *J. Electrochem. Soc.*", **161**, E3248-E3258 (2014)
10. **Z. Liu**, H. Deng, W. Hu, "First-Principles Study of Adsorption and Diffusion Properties of O, H and C Atoms on α -U(001) Surface", *Chin. J. Nonferrous Met.*, **4**, 1160-1167 (2014)

PAPERS UNDER REVIEW

1. F. Soto, **Z. Liu**, P. P. Mukherjee, P. Balbuena, "Elucidating Oligomer-Surface Interactions and Organic Film Growth at a Lithiated Silicon Surface", *Phys. Chem. Chem. Phys.*, under review

CONFERENCE PRESENTATIONS

1. C.-F. Chen, **Z. Liu**,* F. Cano-Banda, A. Hernandez-Guerrero, "A Mesoscale Study of Li₂O₂ Formation in the Lithium-Air Battery Cathode". ASME 2015 International Mechanical Engineering Congress & Exposition, George R. Brown Convention Center, Houston, Texas, USA, Nov 19 (2015)
2. **Z. Liu**,* P. P. Mukherjee, "Influence of Binder Property and Interaction on Electrode Microstructure Formation in Energy Storage". 228th Electrochemical Society Meeting, Phoenix Convention Center, Phoenix, Arizona, USA, Oct 13 (2015)
3. P. P. Mukherjee, **Z. Liu**,* "Physicochemical Interplay in Electrode Processing for Energy Storage"(Invited). 39th International Conference & Exposition on Advanced Ceramics & Composites, Hilton Daytona Beach Resort, Daytona Beach, Florida, USA, Jan 27 (2015)
4. **Z. Liu**,* P. P. Mukherjee, "Probing Active Particle Assembly in Lithium-Ion Battery Electrode Processing". 225th Electrochemical Society Meeting, Hilton Bonnet Creek, Orlando, FL, USA, May 15 (2014)

* denotes the speaker.