LIXIN SUN

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RESEARCH INTERESTS

Understand, predict and design materials for highly efficient heterogenous catalysts, electrochemical energy conversion and storage devices via a combination of simulation modeling techniques.

EDUCATION

2012 – 2018	Ph. D. Massachusetts Institute of Technology, U.S.A. Thesis: Impact of extended defects on ion diffusion and reactivity in binary oxides: assessed by atomistic simulations Adviser: Bilge Yildiz, Prof.
2008 – 2012	Bachelor in Physics, Peking University, China

RESEARCH EXPERIENCE

2018 - Postdoc, Harvard University
Advisor: Boris Kozinsky, Prof. *Materials Intelligence Research Group*

· Develop neural network based dimension reduction algorithms and use them to design collective variables to guide efficient enhanced sampling.

· Develop machine learning force fields to elucidate the dynamical behavior in catalytic reaction on dilute metal alloy and predict accurate reaction rates at finite temperatures

2012 - 2018, Thesis work, MIT
Advisor: Bilge Yildiz, Prof. *Laborotary of Electrochemical Interfaces*

· Elucitate the interplay between extended defects and point defects and how this interplay alters ion diffusion and surface reactivity of binary oxides using multiple advanced computational modeling methods

1. Identify the detrimental effect of dislocations on ionic conductivity in solid oxide fuel cell electrolyte CeO_2 and resistive switching material $SrTiO_3$.
2. Elucidate the impact of dislocations on surface reactions in the Cu/CeO_2 system.
3. Investigate the influence of surface morphological defects on photocatalytic reactivity on TiO_2 nanoparticles.
4. Investigate surface and interface point defect chemistry of CeO_2 , in collaboration with experiments at MIT and Oak Ridge.

SELECTED PUBLICATIONS

1. "Stabilizing single atoms and a lower oxidation state of Cu by a 1/2[110]100 edge dislocation in Cu-CeO_2" L Sun, B Yildiz, *Phys. Rev. Mater.* **3** 025801, 2019
2. "Solubility Limit of Cu and Factors Governing the Reactivity of Cu–CeO2 Assessed from First-Principles Defect Chemistry and Thermodynamics" L Sun, B Yildiz, *The Journal of Physical Chemistry C* **123**, 399-409, 2018
3. "Edge dislocation slows down oxide ion diffusion in doped CeO_2 by segregation of charged defects" L Sun, D Marrocchelli and B Yildiz, *Nat. Comm.*, **6** , 2015

TEACHING EXPERIENCE

2017. Teaching assistant for graduate level *Applid Nuclear Physics*
2016. Supervise MSc student thesis for computational study of surface stability and defect chemistry in $LaMnO_3$

AWARDS

Silver graduate student award from Material Research Society, Spring 2017

Outstanding Teaching Assistant Award from Nuclear Science & Engineering, MIT, 2017

Manson Benedict Award for excellence in academic performance and professional promise in Nuclear Science & Engineering, MIT, 2015

Avery Ashdown Leadership Award, MIT, 2013

Theos J Thompson Memorial Fellowship, MIT, 2013

Manson Benedict (1932) Fellowship, MIT, 2012

LIST OF PUBLICATIONS

4. "The interplay and impact of strain and defect association on the conductivity of rare-earth substituted ceria" GF Harrington, L Sun, B Yildiz, K Sasaki, NH Perry, HL Tuller, *Act. Mater.* **166**, 447-458, 2019
5. "Threshold Catalytic Onset of Carbon Formation on CeO2 during CO2 Electrolysis: Mechanism and Inhibition" J Wang, S Bishop, L Sun, Q Lu, G Vardar, R Bliem, N Tsvetkov, E Crumlin and B Yildiz, *J. Mater. Chem. A* 2019
6. "Accessible switching of electronic defect type in via biaxial strain", YT Chi, M Youssef, L Sun, KJ Van Vliet, B Yildiz, *Physical Review Materials* **5**, 055801, 2018
7. "Strain rate effect on dislocation climb mechanism via self-interstitials" XZ Tang, YF Guo, L Sun, Y Fan, S Yip, B Yildiz, *Materials Science and Engineering: A* **713**, 141-145, 2018
8. "Dislocations in $SrTiO_3$: easy to reduce but not so fast for oxygen transport", D Marrocchelli, L Sun and B Yildiz, *J. Am. Chem. Soc* **137**, 4735-4748, 2015
9. "Improved chemical and electrochemical stability of perovskite oxides with less reducible cations at the surface", Nikolai Tsvetkov, Qiyang Lu, Lixin Sun, Ethan J. Crumlin, and Bilge Yildiz *Nat. Mater.*, **6**,1010-1016, 2016
10. "Self-irradiation of thin SiC nanowires with low-energy ions: a molecular dynamics study", L Sun, C Lan, S Zhao, J Xue and Y Wang, *J. Phys. D: Appl. Phys.*,**45** 135403, 2012
11. "Nanofluidic Pulser Based on Polymer Conical Nanopores" L Wang, L Sun, C Wang, L Chen, L Cao, G Hu, J Xue and Y Wang, *J. Phys. Chem. C*, **46** , 2011