I. 2014 KITCHIN RESEARCH GROUP IN A NUTSHELL

A. Graduated students

Steve Illes, Wenqin You, Meiheng Lu, and Nitish Govindarajan finished their MS degrees! Congratulations!

B. Publications

It looks like six publications this year. We have 5 out for review right now, so next year looks like a good one!

Matthew T. Curnan and John R. Kitchin, Effects of Concentration, Crystal Structure, Magnetism, and Electronic Structure Method on First-Principles Oxygen Vacancy Formation Energy Trends in Perovskites, J. Phys. Chem. C., http://dx.doi.org/10.1021/jp507957n.

Zhongnan Xu and John R. Kitchin, Probing the Coverage Dependence of Site and Adsorbate Configurational Correlations on (111) Surfaces of Late Transition Metals, J. Phys. Chem. C., http://dx.doi.org/10.1021/jp508805h.

Ethan L. Demeter , Shayna L. Hilburg , Newell R. Washburn , Terrence J. Collins , and John R. Kitchin, Electrocatalytic Oxygen Evolution with an Immobilized TAML Activator, Journal of the American Chemical Society, 136(15) 5603-5606 (2014). http://dx.doi.org/10.1021/ja5015986

Robert L. Thompson, Wei Shi, Erik Albenze, Victor A. Kusuma, David Hopkinson, Krishnan Damodaran, Anita S. Lee, John R. Kitchin, David R. Luebke and Hunaid Nulwala, Probing the effect of electron donation on CO2 absorbing 1,2,3-triazolide ionic liquids, RSC Advances, 4 (25), 12748-12755 (2014). http://dx.doi.org/10.1039/C3RA47097K.

Mehta, Prateek; Salvador, Paul; Kitchin, John, Identifying Potential BO2 Oxide Polymorphs for Epitaxial Growth Candidates", ACS Applied Materials and Interfaces, 6(5), 3630-3639 (2014). http://pubs.acs.org/doi/full/10.1021/am4059149.

Zhongnan Xu and John R Kitchin, Relating the Electronic Structure and Reactivity of the 3d Transition Metal Monoxide Surfaces, Catalysis Communications, 52, 60-64 (2014), http://dx.doi.org/10.1016/j.catcom.2013.10.028.

C. Presentations

John Kitchin, Jacob Boes, Gamze Gumuslu, James Miller, Andrew Gellman, Bulk Composition Dependent H2 Dissociative Adsorption Energies on CuxPd1-x Alloy Surfaces, U. Missouri, Department of Chemical Engineering, September 2014.

John Kitchin, The next evolution in water oxidation, Department of Materials Science, Duke University, March 2014.

John Kitchin, Jacob Boes, Gamze Gumuslu, James Miller, Andrew Gellman, Bulk Composition Dependent H2 Dissociative Adsorption Energies on CuxPd1-x Alloy Surfaces Department of Energy - Basic Energy Science Catalysis Program meeting, July 2014.

Jacob R. Boes and John R. Kitchin, Estimating Bulk Composition Dependent H2 Dissociative Adsorption Energies on CuxPd1-x Alloy (111) Surfaces, AICHE Atlanta, Nov 2014.

Zhongnan Xu and John R. Kitchin, Coverage-Dependent Site and Adsorbate Configurational Correlations on (111) Surfaces of Late Transition Metals, AICHE Atlanta, Nov 2014.

Matthew Curnan and John R. Kitchin, Prediction of Phase Stability and Transition Pressures in BO2 (B = Ti, V, Ru, Ir) Polymorphs Using DFT+U and Self-Consistent Linear Response Theory, AICHE Atlanta, Nov 2014.

John Kitchin, A success story in using Python in a graduate chemical engineering course, SciPy 2014, June 2014. `https://www.youtube.com/watch?v=IsSMs-4GlT8`

D. Recognitions

Professor Kitchin awarded the Philip L. Dowd Fellowship Award (link).

Mehak Chawla awarded a Prengle Fellowship (link).