

Floating Island - ISDP Group 33

Ben Frazer*

February 28, 2022

Contents

1	Section one	1
2	Bibliography	1

1 Section one

- [1]
- [2]
- [3]
- [4]
- [5]
- [6]
- [7]
- [8]
- [9]
- [10]
- [11]

2 Bibliography

References

- [1] Alexander P. Hallenbeck and John R. Kitchin. Effects of O_2 and SO_2 on the capture capacity of a primary-amine based polymeric CO_2 sorbent. *Industrial & Engineering Chemistry*, 107:94–107, 2013.
- [2] Prateek Mehta, Paul A. Salvador, and John R. Kitchin. Identifying potential BO_2 oxide polymorphs for epitaxial growth candidates. *ACS Appl. Mater. Interfaces*, 6(5):3630–3639, 2014.
- [3] 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.
- [4] 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*, 118(44):25597–25602, 2014.

*2704250F@student.gla.ac.uk

- [5] Spencer D. Miller, Vladimir V. Pushkarev, Andrew J. Gellman, and John R. Kitchin. Simulating temperature programmed desorption of oxygen on Pt(111) using DFT derived coverage dependent desorption barriers. *Topics in Catalysis*, 57(1-4):106–117, 2014.
- [6] 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. *The Journal of Physical Chemistry C*, 118(49):28776–28790, 2014.
- [7] Jacob R. Boes, Gamze Gumuslu, James B. Miller, Andrew J. Gellman, and John R. Kitchin. Estimating bulk-composition-dependent H₂ adsorption energies on Cu_xPd_{1-x}alloy(111)surfaces. *ACSCatalysis*, 5 : 1020 – –1026, 2015.
- [8] Zhongnan Xu, Jan Rossmeisl, and John R. Kitchin. A linear response DFT+U study of trends in the oxygen evolution activity of transition metal rutile dioxides. *The Journal of Physical Chemistry C*, 119(9):4827–4833, 2015.
- [9] Zhongnan Xu and John R. Kitchin. Relationships between the surface electronic and chemical properties of doped 4d and 5d late transition metal dioxides. *The Journal of Chemical Physics*, 142(10):104703, 2015.
- [10] Jacob R. Boes, Mitchell C. Groenenboom, John A. Keith, and John R. Kitchin. Neural network and Reaxff comparison for Au properties. *Int. J. Quantum Chem.*, 116(13):979–987, 2016.
- [11] Jacob R. Boes and John R. Kitchin. Neural network predictions of oxygen interactions on a dynamic Pd surface. *Molecular Simulation*, pages 1–9, 2017.