

Electronic Supplementary Information

Hydrogen Desorption from the Surface and Subsurface of Cobalt

Ryan A. Ciufu^{ab}, Sungmin Han^a, Michael E. Floto^a, J. Ehren Eichler^a, Graeme Henkelman^{*ab}, and C. Buddie Mullins^{*ac}

^{a.} Department of Chemistry, University of Texas at Austin, Austin, Texas 78712 United States.

^{b.} The Oden Institute for Computational Engineering and Science, University of Texas at Austin, Austin, Texas 78712, United States.

^{c.} The McKetta Department of Chemical Engineering, Texas Materials Institute, Center for Electrochemistry, University of Texas at Austin, Austin, Texas 78712, United States.

Details on Microkinetic Modelling.

Temperature programmed desorption (TPD) spectra were simulated using the desorption energies calculated from density functional theory (DFT). For associative desorption of hydrogen, a linear fit to the coverage dependent desorption energies (Table 1) was used (Figure S1). For associative hydrogen desorption from surface sites above a subsurface site, a desorption energy of 0.82 eV was used (Table 1, $\theta = 1.0$, $\theta_{\text{subsurface}} = 0.25$). After desorption of hydrogen from above a subsurface site, the subsurface hydrogen was allowed to resurface. Once all subsurface hydrogen was depleted, desorption followed the coverage dependent rate.

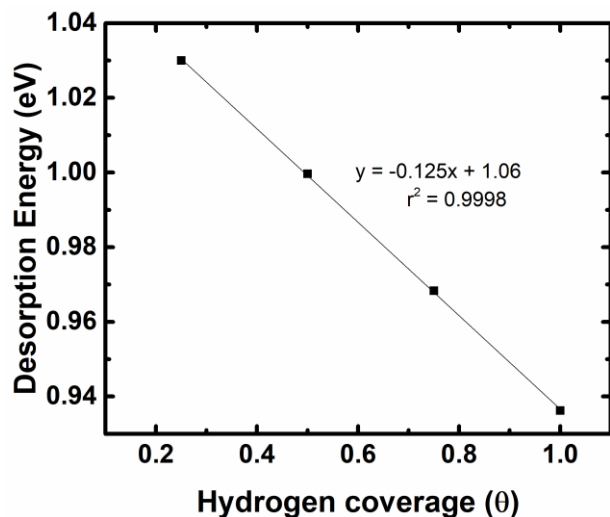


Figure S1. Linear fit for coverage dependent hydrogen desorption energies used for microkinetic analysis.