

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Oxygen Evolution Electrocatalysis on Cobalt Oxide surfaces¹ MICHAL BAJDICH, JCAP-North, LBL, Berkeley, CA 94720, JENS K. NORSKOV, SUNCAT, SLAC, Stanford, CA 94025, MONICA GARCÍA-MOTA, Department of Chemical Engineering, Stanford University, Stanford, CA 94305, ALEXIS T. BELL, JCAP-North, LBL, Berkeley, CA 94720 — The oxidation of water for hydrogen production using sunlight is of high importance to photo-fuel cell research. The electrochemical approach via heterogeneous catalysis to water splitting is a very promising route. The key challenge of this method lies in reduction of the losses, i.e., over-potential, for the oxygen evolution reaction (OER) on the anode. In this work, we investigate the dependence of theoretical over-potential of OER on type of anode by applying standard density functional theory (DFT). We attempt to explain recent experimental observation of enhanced activity on gold supported Cobalt Oxide surfaces [1]. We explore variety of possible CoO structures and associated surfaces which could emerge under operating conditions of catalyst. Finally, we also explore the influence of environment and admixtures of CoO with other elements.

[1] B.S. Yeo, A.T. Bell, *AT*, *J. Am. Chem. Soc.*, 133, 5587-5593 (2011).

¹support from Joint Center for Artificial Photosynthesis (heterogeneous catalysis)

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Date submitted: 08 Dec 2011

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