Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Al-Air Batteries: Fundamental Thermodynamic Limitations from First Principles Theory[1] LEANNE D. CHEN, JENS K. NOERSKOV, ALAN C. LUNTZ, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory/Stanford University — The Al-air battery possesses high theoretical specific energy (4140 Wh/kg) and is therefore an attractive candidate for vehicle propulsion applications. However, the experimentally observed open-circuit potential is much lower than what thermodynamics predicts, and this potential loss is widely believed to be an effect of corrosion. We present a detailed study of the Al-air battery using density functional theory. The results suggest that the difference between bulk thermodynamic and surface potentials is due to both the effects of asymmetry in multi-electron transfer reactions that define the anodic dissolution of Al and, more importantly, a large chemical step inherent to the formation of bulk Al(OH)3 from surface intermediates. The former results in an energy loss of 3%, while the latter accounts for 14−29% of the total thermodynamic energy depending on the surface site where dissolution occurs. Therefore, the maximum open-circuit potential of the Al anode is only −1.87 V vs. SHE in the absence of thermal excitations, contrary to −2.34 V predicted by bulk thermodynamics at pH 14.6. This is a fundamental limitation of the system and governs the maximum output potential, which cannot be improved even if corrosion effects were completely suppressed.

[1] Supported by the Natural Sciences and Engineering Research Council of Canada and the ReLiable Project (#11-116792) funded by the Danish Council for Strategic Research

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Date submitted: 11 Nov 2014 Electronic form version 1.4