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**First principle studies of the oxygen reduction reaction on the CrN electrocatalyst** SERGEY STOLBOV, University of Central Florida — These fuel cells offer great advantages for various applications, but severe obstacles remain to their large scale implementation. The Pt-based catalysts, used in both electrodes make them unacceptably expensive. Furthermore, the low rate of the oxygen reduction reaction (ORR) on the Pt cathode significantly reduces efficiency of the device. In this work, ORR on alternative CrN electrocatalyst has been studied from first principles. It is found that, in contrast to Pt, oxygen molecules dissociate spontaneously on the CrN surfaces, which switch on simple 1-electron reduction mechanism. Based on the adsorption energy calculations the free energies of intermediates were obtained as functions of the electrode potential. This diagram explain a relatively high rate of ORR obtained experimentally [1] for this material. The effects of coverage and co-adsorbates have been also studied.

[1] H. Zhong, et al., Appl. Phys. Lett. 91, 163103 (2007).

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