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**First-Principles Studies of Electric Field Effects in Heterogeneous Catalysis: $NH_3$on Ru(0001)** AARON SISTO, Department of Mechanical Engineering, Purdue University, West Lafayette, IN 47906, ALEXEY ZAYAK, JEFFREY NEATON, Molecular Foundry, LBNL, Berkeley, CA 94720 — The catalytic dissociation of $NH_3$ has been the focus of recent studies due to the prospect of efficient hydrogen storage and generation. The effects of a static electric field on the surface electronic structure and energy barriers of reactions are examined using density functional theory calculations with gradient corrections. It is found that the interaction strength between the adsorbate and surface can be tuned based on the magnitude and polarity of the field, as evidenced by a field-induced shift of the d-electron band. Correspondingly, energy barriers along minimum energy pathways for desorption and dissociation reactions are significantly affected by the change in substrate-adsorbate interaction. It is concluded that the application of an electric field enhances the catalytic performance of Ru through increased activity and selectivity of $NH_3$ dissociation. We acknowledge support from DOE, DOE CSGF Fellowship. Computational resources provided by NERSC.

Aaron Sisto
Department of Mechanical Engineering,
Purdue University, West Lafayette, IN 47906

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