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Electric Field-Induced Dissociation of NH_3 on Ru(0001) from First Principles[1] AARON SISTO, Department of Mechanical Engineering, Purdue University, West Lafayette, IN 47906, ALEXEY T. ZAYAK, Molecular Foundry, LBNL, Berkeley, CA 94720, Department of Electrical Engineering and Computer Sciences, UC Berkeley, CA 94720, USA, JEFFREY B. NEATON, Molecular Foundry, LBNL, Berkeley, CA 94720 — Recent experimental evidence suggests that an applied electric field from an STM tip can induce rapid dissociation of NH3 on a Ru(0001) surface. Here, density functional theory calculations, within the generalized gradient approximation, are used to understand the experimental observations and develop a clear picture of this complex reaction. The desorption and dissociation thresholds are found to occur at E=-0.06 V/Åand E=0.12 V/Å, respectively, in good agreement with experiment. Calculation of the energy barrier along a potential reaction pathway indicates a decrease of 0.50 eV in the barrier at the dissociation threshold. A field-induced softening of the ammonia umbrella mode is found to explain the initial dissociation. It is concluded that an applied electric field greatly enhances the dissociation reaction rate through a reduction of the reaction energy barrier.

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