Computational Chemistry

Homework 1

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1. Maier S, Stass I, Feng X, Sisto A, Zayak A, Neaton J, Salmeron M. J. Phys. Chem. C, 119, 19, (2015) "Dehydrogenation of ammonia on Ru(0001) by electronic excitations"

2. The authors seek to understand the effect of an electric field on ammonia decomposition at the single-molecule level. They explain that thermal activation of ammonia decomposition populates all vibrational modes of the ammonia molecules, but all of these modes might not contribute to lowering activation energies. A goal of this work was to identify which excitations are the most important for this particular reaction.

3. The activation energies for three ammonia decomposition steps were computed as functions of the strength of an applied electric field. The relative changes in these barriers showed which mechanisms were affected most strongly by the electric field. The authors conclude that there is a combination of barrier changes that must occur for the reaction to proceed and that N-H dissociation barriers change the most with respect to electric field voltage.