A Computational Study of Hydrogen Production Through Water-Splitting

Deacon J. Lile, Karl Kirschner, and George Shields
Hamilton College Department of Chemistry, Clinton, NY, 13323

The use of solar energy in the production of hydrogen and oxygen through water splitting shows promise as an environmentally friendly source of hydrogen. This uphill reaction has been studied extensively because of hydrogen's potential as a "green" energy source. To date, the vast majority of research involving water splitting uses various photo-catalysts that harness solar energy to create a potential, which is then used to split water through a series of redox reactions. This project is a preliminary exploration of a new method for hydrogen production; two water molecules are split directly into hydrogen and oxygen gas via a one step mechanism. Computations were conducted using the MP2 and CCSD(T) levels of theory. These computations clarify the thermodynamics of this mechanism and the possible catalytic effects of various polar groups. These theoretical studies were used to determine the Gibbs free energy of the reactants, products and each structure along the reaction pathway (including the transition states). By mapping the thermodynamics of this entire reaction, we were able to determine that our mechanism, with an appropriate catalyst, has the potential to drive this reaction uphill using only solar energy.