CALIFORNIA STATE SCIENCE FAIR
2012 PROJECT SUMMARY

Name(s)
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Project Number
S0611

Project Title
Catalytic Conundrum 2: A Computational Method of Finding Cost-Effective Replacements for Platinum as Fuel Cell Catalysts

Abstract

Objectives/Goals
Currently, energy is one of the primary concerns for the world. Many alternatives to the combustion of fossil fuels have been proposed, one of which is hydrogen fuel cell technology. It is efficient but very expensive. Much of this cost can be attributed to using a platinum (Pt) catalyst. Replacing the catalyst with a cheaper metal can make fuel cells a cheaper alternative to the present system. My experiment was conducted to find the viability of certain alternative catalysts by computationally modeling the reaction of those catalysts and comparing their reaction pathways and enthalpies to that of Pt. Based on strong chemical similarities to Pt, I hypothesized that palladium (Pd) and nickel (Ni) would make strong candidates for a less expensive replacement catalyst and would have similar exothermic reaction pathways.

Methods/Materials
My experiment was conducted using density functional theory calculations in Gaussian 09. I utilized the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) functional with the Los Alamos National Laboratory 2-double-z (LANL2dz) basis set for Pt, Pd, and Ni and the 6-31G basis set for hydrogen and oxygen. Dimers of each metal and several alternate spin states and transition states were tested. Each configuration was recorded along with its energy and placed into an estimated reaction pathway for both the anode and cathode side of the fuel cell reaction.

Results
For Pt, the reaction at the anode is largely endothermic with a comparative molecular energy of 768.93 kcal/mol. The reaction at the cathode was exothermic with a comparative molecular energy of -1035.31 kcal/mol. Overall, the reaction is exothermic. Pd and Ni show a similar trend. The reaction pathway for each is remarkably similar to that of Pt. The pathways indicate possible exothermic reactions, but alternate spin states and transition states need to be tested in order to confirm this observation.

Conclusions/Discussion
I initially hypothesized that Pd and Ni would both have a similar reaction pathway to Pt and that the reaction for both would be exothermic. Due to the lack of some alternate spin states and transition states, this hypothesis could not effectively be supported or rejected. Based on the data I have thus far, my hypothesis is supported, but additional testing is needed to confirm this. I will be continually running these tests and wish to test other possible catalysts as well.

Summary Statement
My experiment uses computational chemistry to model the activation of hydrogen on various metals (platinum, palladium, nickel) in an effort to discover an economically effective source for catalysts in proton exchange membrane fuel cells.

Help Received
Dr. Tiffany Pawluk of CSU Bakersfield provided access to Gaussian 09; My mom provided transportation.