CALIFORNIA STATE SCIENCE FAIR
2013 PROJECT SUMMARY

Name(s)

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Project Number

S0606

Project Title

Catalytic Conundrum 3: Effect of Cluster Size and Isomers on Activation of H2 on Pt Particles in PEM Fuel Cell Reaction

Abstract

Objectives/Goals

Fuel cell technology is about 60% efficient but costs around $1500/kW. Optimizing the energy output of the platinum catalyst by altering the individual structures could lower the cost. My experiment observes the effect of cluster size and isomers on the activation of hydrogen on platinum clusters in a fuel cell reaction. Based on the instability of more complex structures in a chemical reaction, I hypothesized that smaller and simpler platinum structures would have higher catalytic properties and yield higher energies.

Methods/Materials

My experiment was conducted using density functional theory calculations in Gaussian 09. I utilized the Becke, 3-parameter, Lee-Yang-Parr functional with the Los Alamos National Laboratory 2-double-z basis set for platinum and the polarized and diffused 6-31G basis set for hydrogen and oxygen. Monomers and dimers of platinum and several alternate spin states and transition states were tested. Testing for trimers and tetramers are currently ongoing. Each configuration was recorded along with its energy and placed into an estimated reaction pathway for both the anode and cathode side of the reaction.

Results

The catalysis of hydrogen on the anode on single platinum atoms was endothermic. Along the reaction pathway it switches between the singlet and triplet spin states and requires 817.63 kcal/mol. Along the cathode, the reaction is exothermic, yielding 1180.29 kcal/mol. The overall fuel cell reaction on single platinum atoms is exothermic, producing 362.66 kcal/mol. For dimers, the reaction at the anode is endothermic with a comparative molecular energy of 768.93 kcal/mol. The reaction at the cathode was exothermic with a comparative molecular energy of -1055.42 kcal/mol. Overall, the reaction on the dimer configuration is exothermic with a yield of 266.38 kcal/mol.

Conclusions/Discussion

I initially hypothesized that smaller and simpler compounds would be more effective at the activation of hydrogen on platinum in a fuel cell system. As of now, my data supports my hypothesis. The reaction on a single atom produced 96.28 kcal/mol more than the reaction on two platinum atoms. In order to effectively confirm my hypothesis, trimers and tetramers, along with their isomers, need to be tested and compared to my other results. Further calculations will be made to compare my results with experimental data from actual fuel cells. There will be a updated abstract with my project.

Summary Statement

My experiment uses computational chemistry to study the effect of cluster size and isomers on the activation of hydrogen on platinum clusters in a proton exchange membrane fuel cell reaction.

Help Received

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