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Improving modeled experiments to allow development of new catalysts

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INTRODUCTION

In order to make sustainable materials like lactic acid based plastics available on a commercial scale, an efficient conversion of the bio-mass is needed. Traditionally lactic acid has been produced from sugars using fermentation, but new methods based on heterogeneous catalysts are being developed[1]. In order to improve the conversion rate, a lot of candidate catalysts need to be tested. Traditionally this has only been possible through physical experiments. In this project we have developed a method to improve the accuracy of the parameterization for a modeling technique called Reactive Force Fields (ReaxFF) that will allow these experiments to be performed on a computer rather than in a lab.

THEORY AND METHODS

A reactive force field like ReaxFF is used to calculate the most likely structure of a molecule by minimizing the energy level in the molecule. The force field is given as input the position of the atoms, but no bonds. These are instead calculated using the given parameters (e.g. the energy level of a C-C bond). The parameters as a whole define all the energy levels of the various bonds, the bond angles and torsions. A parameterization is to define all of these parameters to match the expected energy levels. The parameterization can be viewed as a vector or position in a multidimensional space. By assigning a penalty to each position in this space, we can reduce the problem to a search in the multidimensional space for the position with the lowest penalty. To do this, we use the meta-heuristic optimization called the Particle Swarm Optimization.

RESULTS

In the project we demonstrate that the optimization technique works by performing a parameterization for smaller molecules consisting only of H and C atoms. In the project we also demonstrate that the method can be extended to larger scale parameterizations and develop a parallelized version to reduce the computing time involved with running the optimization.

[1] Holm, M. S, et. al, (April 30th 2010). Conversion of Sugars to Lactic Acid Derivatives Using Hetorogeneous Zeotyp Catalysts, *Science, Vol 328,* 602-603