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Catalysts for African Development and Advancement [CADA]

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The twin problems of electricity shortage and limited access to clean drinking water in Africa can be solved by the development of catalysts. Abundant catalysts that can facilitate the splitting of water into hydrogen gas (and oxygen gas) are required as well as cheaper catalysts that can be used in fuel cells to produce electricity by the oxidation of hydrogen. An important by product of the fuel cell is clean water from the combination of hydrogen and oxygen. Thus, even dirty water can be used to produce electricity and clean water. While platinum and platinum-ruthenium alloys work as catalysts in fuel cells, they are costly and cheap and abundant alternatives are needed. The goal of this work is to understand the mechanism of action of these expensive catalysts as a guide to developing alternative cheap and abundant catalysts for fuel cells. Semi-empirical molecular dynamics (SEMD) simulation will be used to study the oxidation of hydrogen by platinum and comparisons made with the same process but in the presence of a recently discovered catalyst Fe(PO3)2. Preliminary SEMD simulations of possible catalysts for photocatalytic water splitting will also be presented.

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