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Challenges in multi-scale modeling of fuel electro-oxidation for fuel cell applications

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The high-cost of materials and efficiency limitations chemical fuel cells currently have is a topic of primary concern. Many industries are currently focusing on PEM fuel cells engineering and design for improved performance and durability, and reduced cost. This situation has led to an urgent need for understanding, predicting, and optimizing the various transport and electrochemical processes that occur in PEM fuel cells, where modeling has played a key role.

Bioelectrochemical generation of power by enzymes has also been considered. Enzymatic fuel cells have been reported to have power output and stability limitations; which are restricting the use of this kind of fuel cell to small electronic devices. However, understanding how enzymes carry out oxidation processes could lead to the development of new synthetic bio-inspired chemical catalysts that could impact the use of cheap fuels, such as methanol.

Challenges associated to a multi-scale modeling approach to model fuel electro-oxidation in PEM and bio fuel cells are discussed here. A combination of tools involving Density Functional Theory, Transition State Theory, Molecular Mechanics and Kinetic Monte Carlo are combined in order to model fuel electro-oxidation. Information regarding energy barriers and pre-exponential factors needed to determine reaction rates are obtained from DFT and TST respectively. These microscopic reaction rates are then provided as inputs in the kMC program, and the fuel oxidation process is modeled on a 2-D reactive surface representing the catalyst.

Biography

Daniela Mainardi is an Associate Professor and Program Chair of Chemical Engineering at Louisiana Tech University; currently holding the Thomas C. & Nelda M. Jeffery Professorship in Chemical Engineering. Mainardi has extensive experience in a large variety of multi-scale molecular simulation tools and has conducted research on different and complementary nano- and bio-technology-related topics with applications to transport and catalysis. Mainardi has received the NSF-CAREER award in 2005 on Modified-Methanol Dehydrogenase Enzymatic Catalysts For Fuel Cell Devices. Mainardi is a senior member of the American Institute of Chemical Engineers (AIChE) and the current AIChE Transport and Energy Processes Division Chair.

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