

## **Simulation of Reaction and Transport Processes in Fuel Cell Catalysts and Membranes**

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We will report here progress in using multiple paradigms for simulations of new materials for catalysts and membranes toward improved fuel cell performance. Dramatically improving the performance of fuel cells systems with their complex heterogeneous structures involving electrocatalysts, proton conducting membrane, reactant, and interfaces between them requires understanding the fundamental chemical, electrochemical, and physical phenomena at the heart of these complex materials and relating these fundamentals to the properties and performance of the membrane-electrode assembly.

Our goal is to develop predictive models that can be used to estimate the changes in performance upon changes in the design and which can be used to monitor performance of working fuel cells. Our strategy is to start with first principles quantum mechanics and to develop overlapping simulation methodologies in which quantum mechanics is used to train a reactive force field that can be applied for large-scale (many 1000s of atoms) molecular dynamics simulations while retaining the accuracy of quantum mechanics.

Our expectation is that this model would enable the conception, synthesis, fabrication, characterization, and development of advanced materials and structures for fuel cells. We illustrate here some of the progress toward this goal.