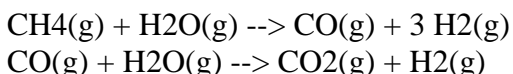


Theoretical Catalyst Design for Hydrogen Fuel Production

Wayne Blaylock, Greg Beran, and William Green, MIT
De Chen and Anders Holmen, Norwegian University of Science and Technology

The problems associated with automobile pollution, from releasing greenhouse gases that contribute to global warming to the adverse health effects of photochemical smog, are well known. For this reason, researchers around the world are working towards the hydrogen-powered automobile and other aspects of a hydrogen economy. One major source of hydrogen fuel currently is from the steam reformation of natural gas:



the first step of which is typically nickel-catalyzed. Modern reactor systems are being developed which enable the in-situ separation of the H₂ and CO₂ gases at centralized plants and allow sequestration of the CO₂. The hydrogen fuel can then be distributed to end-users for emission-free use. Unfortunately, under industrial conditions, the nickel catalyst is prone to carbon formation (coking) which encapsulates and deactivates the catalyst.

In order to improve the feasibility of this process, we are searching for novel catalysts that are more resistant to carbon formation using the techniques of quantum chemistry. As the first step, we are constructing the first, comprehensive ab initio model for steam reforming on nickel surfaces using density functional theory with periodic boundary conditions. Using this model to identify the key steps in the process, we can understand how different catalysts affect the surface chemistry and inhibit carbon formation. These kinetic models will be incorporated into a reactor model to simulate the experimental system developed by our collaborators. In turn, our collaborators will synthesize and test the catalysts we have identified in their reactor.