Nickel Particles as Catalysts in Hydrocarbon Chemistry
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Nickel particles have been studied as catalysts for various aspects of hydrocarbon chemistry for several decades because of their significance in several industrial processes. Of particular interest are the steam reforming process which converts methane and water into synthesis gas (carbon monoxide and hydrogen), the Fischer-Tropsch formation of higher order hydrocarbons and in recent years the formation and growth of carbon nanotubes. Surface science experiments have primarily focused on the chemisorption of methane on nickel particles as the critical step in these catalytic processes, however an understanding of how various products are formed requires a detailed knowledge of the chemistry that takes place following chemisorption.

To gain insight into this surface chemistry we have used periodic DFT to study the free energies of hydrocarbons bound to a variety of nickel surface sites as well as the barriers for hydrocarbon reactions on the Ni111 surface. These \textit{ab initio} results are compatible with and explain experimental observations.

Furthermore, we have used these DFT results to train the parameters for the reactive force field ReaxFF. We use this ReaxFF description of hydrocarbon chemistry in the presence of nickel to explore more complex aspects of hydrocarbon chemistry on nickel catalyst particles. In particular we explore various aspects of the carbon nanotube growth process, including the production of activated carbon species from methane initially chemisorbed on the surface, the addition of the activated carbon species to a growing nanotube edge and the formation carbon ring structures believed to be the precursors of nanotubes.