DFT-based Design of Nano Alloy Catalysts: Surface d Orbital Occupancy and Lattice Strain Engineering

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The hydrogen and fuel cells have received much attention in recent years as a promising alternative to fossil fuel-based power generation. One of the major barriers to their commercialization is the low efficiency of catalysts in running the fuel cell and hydrogen production system. Thus, there exists great interest in developing alternative hydrogen and fuel cell catalysts. The essential part in the development of high-performance catalysts is to properly tailor the physical and chemical properties of catalysts. However, a detailed understanding of how to control the properties of such catalysts is still lacking, despite its importance in designing and developing novel and cost effective catalysts. This is in large part due to the difficulty of direct characterization. Alternatively, quantum mechanics-based DFT (Density functional theory) approaches have emerged as the powerful and flexible means to unravel the fundamental principles of hydrogen and fuel cell catalysts, which may allow the new finding of the breakthrough catalysts. In this talk, using DFT and machine-learning methods, I will present the design of nano alloy catalysts for hydrogen and fuel cell applications.