Ab initio Simulations for Membrane based Hydrogen Separation Processes

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Hydrogen used as a fuel for hydrogen fuel cells can be obtained mainly in the process of treating hydrocarbon materials such as petroleum. Hydrogen obtained from hydrocarbons is mixed in various byproducts. In order to use it as a fuel for a fuel cell, a pretreatment process for purifying hydrogen is essential. Amorphous silica (a-SiO2) typically has micropores of 0.5-2 nm in diameter with a narrow pore size distribution, which allows selective permeation of H2 from complex gas mixtures from methane steam reforming processes. Despite of the many advantages, porous a-SiO2 membranes exhibit poor hydrothermal stability in moist atmospheres, which is the major problem for their application in H2 production processes. One possible solution for improving the hydrothermal stability of the a-SiO2 membranes is doping of transition metals, such as Aluminum, titanium, cobalt, and nickel. However, little is known about the fundamental causes of such stabilization of the doped a-SiO2.