Metal Doping Effect on the Hydrothermal Stability of Porous Amorphous Silica for Hydrogen Separation Membranes

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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. In this work, we apply density-functional theory calculations on a model a-SiO2 surface and investigate how the metal-doping enhance the poor hydrothermal stability of the porous a-SiO2 membrane surfaces. Subsequent examination of surface electronic structures provides a theoretical support to the direct correlation between the modified surface electronic structures and the promoted hydrothermal stabilities.