Growth Behavior and Hydrogen Evolution Reaction Activity Trends of Transition Metal Sulfides Embedded in Nanoporous Carbons

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Metal sulfide-based nanostructured materials have emerged as promising non-precious metal catalysts for hydrogen evolution reaction (HER). The understanding of nanoscale size-dependent catalytic activities can provide the scientific basis for the design of advanced catalysts. However, nanoscale size effects in metal sulfide-based HER catalysts have not yet been established fully, due to the synthetic difficulty in precisely controlling the size on the nanometer scale in the basal and edge plane directions. In this talk, we will present the synthesis of MS_2 (M = Mo or W) nanoparticles (NPs) embedded in nanoporous carbons (MS_2@OMC) by limiting their growth space in nanoscale. Experimental and theoretical results revealed that vertical growth is favored in MoS_2 to generate multiply stacked MoS_2 NPs, whereas the horizontal growth is preferred in WS_2 to yield monolayer NPs. We established that the turnover frequency (TOF) of layer number-controlled MoS_2@OMC increases with decreased layer numbers in MoS_2. The TOF of monolayer WS_2@OMC with controlled size increases with increasing atomic ratio of the basal and edge atoms in WS_2.