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Design of Beta Phase Mo_2C Catalyst for Hydrogen Evolution Reaction via Nanoparticle Morphology Control: Insights from First Principles Methods and Kinetic Modeling TIMOTHY T. YANG, WISSAM A. SAIDI, University of Pittsburgh — Transition metal carbides, in particular β-phase Mo_2Cs, are garnering increased attention as hydrogen evolution reaction (HER) catalysts due to their favorable synthesis conditions, stability and high catalytic efficiency. We use a thermodynamic approach in conjunction with density functional theory and a kinetic model of exchange current density to systematically study the HER activity of β-Mo_2C under different experimental conditions. We show that (011) surface has the highest HER activity because this surface does not expose strong Mo-based hydrogen adsorption sites. We give definite maps between nanoparticle morphologies and experimental synthesis conditions, and show that an increase of hydrogen partial pressure during synthesis can expose (011) surface up to 90 percent, which increase by extension the HER activity. The volcano plot shows that under these optimum conditions, the NP exchange current densities can be increased by more than one order to 10^{-5} A/cm^2, that is only slightly smaller than that of Pt (111).

Wissam A. Saidi
University of Pittsburgh

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