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Enhancing the Hydrogen Activation Reaction of Nonprecious Metal Substrates via Confined Catalysis Underneath 2D Materials[1] YINONG ZHOU, Univ. of Sci. and Tech. of China, Univ. of Utah*, WEI CHEN, PING CUI, JIANG ZENG, ZHUONAN LIN, ICQD, Univ. of Sci. and Tech. of China, FENG LIU, Univ. of Utah, EFTHIMIOS KAXIRAS, Harvard Univ., ZHENYU ZHANG, ICQD, Univ. of Sci. and Tech. of China — In the hydrogen evolution reaction (HER), the reactivity as a function of the H adsorption energy on different metal substrates follows a well-known volcano curve, peaked at Pt. The goal of turning nonprecious metals into efficient catalysts is a fundamental challenge. Here, we present DFT calculation results toward achieving this goal by exploiting the synergistic power of marginal and confined catalysis. We first show that the volcano curve stays qualitatively intact when van der Waals attraction is included. We then show that the H adsorption energy is lowered when H is confined between graphene and the metal surfaces, with Ni exhibiting the largest change. In particular, the graphene-modified volcano curve peaks around Ni, and the corresponding HER rate is comparable to that of bare Pt. These findings demonstrate that graphene-covered Ni is an appealing effective, stable, and economical catalytic platform for HER. The above studies are being also extended to MoS_2-covered metal substrates, which may peak at a different metal in the volcano curve.

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