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First-principles study on two dimensional dichalcogenides for hydrogen production

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Hydrogen is a promising candidate for the clean energy carrier that may replace fossil fuels. For the production of hydrogen, water splitting with efficient catalysts has been intensively studied over the past decades. Platinum, which is known to be the best catalyst for water splitting, is too expensive to be used in large-scale applications. Therefore, numerous earth-abundant materials have been investigated as a replacement of Pt. Recently, transition metal dicalcogenides (TMDs), most notably MoS2, are receiving a great deal of attention as a novel catalyst for water splitting. Although the basal plane of TMDs are efficient as catalysts, it was found recently that the sulfur vacancy in MoS2 can increase the catalytic activity for hydrogen evolution.
In this presentation, motivated by the previous work, we explore the detailed mechanism for hydrogen production from the sulfur vacancy in MoS2 and calculate the activation energies along the reaction path. Furthermore, we evaluate the catalytic efficiency of vacancy sites in various TMDs and suggest TMDs that may show high catalytic effects in hydrogen evolution reaction.

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