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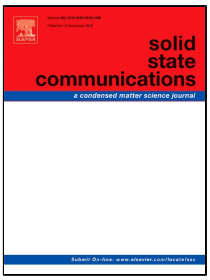

Theoretical investigation of platinum-like catalysts of molybdenum carbides for hydrogen evolution reaction

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Theoretical investigation of platinum-like catalysts of molybdenum carbides for hydrogen evolution reaction

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Abstract:

Developing high-active, stable and low-cost hydrogen evolution reaction (HER) catalysts is essential for industrial hydrogen production. Herein, a systematic study of the structures of molybdenum carbides and the related HER mechanism have been carried out based on density functional theory (DFT) calculations. The electronic properties and surface energies of three typical crystals of molybdenum carbides, i.e., α-MoC, β-MoC and γ-Mo_2C, have been analyzed. It is shown that all the systems considered exhibit metallic behavior, among which the β-MoC (110) plane is the most active facet with the largest surface energy (3.159 $J \cdot m^{-2}$). By comparing the Gibbs free energies, $\Delta G(H)$, we find that the (111) surface of β-MoC has the smallest $\Delta G(H)$ of 0.089 eV, which is even superior than Pt-like catalysts, V_8C_7 (-0.114 eV), VC (-0.191 eV) or MoO_2 (0.15 eV).

Key words : DFT calculations, Molybdenum carbides , Pt-like catalysts , Hydrogen evolution reaction

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