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Kinetic study and simulation of molybdenum borides for hydrogen evolution reaction

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ABSTRACT

This paper presented the kinetic study of molybdenum borides via the Volmer-Heyrovsky-Tafel (V-H-T) mechanistic steps for hydrogen evolution reaction (HER). A theoretical approach was carried out to investigate the kinetic properties of several molybdenum boride materials for HER in 0.5 M H2SO4. Our findings offer definitive proof that the simulated results show that B, Mo, Mo2B, and α-MoB, proceed through V-H mechanistic steps (slower kinetics) while β-MoB and MoB2 exhibit V-H-T mechanistic steps with higher kinetics. The kinetic parameters were determined in terms of the standard rate constant parameters for the Volmer step (kV, k-V), Heyrovsky step (kH, k-H), and rate constant for the Tafel step (kT, k-T). The simulation was able to predict the overpotential at 10 mA/cm2, η10 recorded at approximately 780, 585, 480, 350, 310, and 300 mV for B, Mo, Mo2B, α-MoB, β-MoB, and MoB2 respectively. Based on these findings, the adopted mathematical model shows good coherency to the experimental findings. The simulation work provides a good numerical estimation of the characteristics of the electrocatalyst for HER. This paper successfully elucidated the reaction mechanisms (V-H-T steps) and understood the rate-limiting steps involved in the HER process on Mo-B materials.

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1. INTRODUCTION

Developing highly efficient HER low-cost electrocatalysts is of utmost importance to realize hydrogen economy. Earth's abundant compounds such as carbons have attracted tremendous research interest. Among them, molybdenum carbides have exhibited great potential catalytic properties [1]–[3]. Recent studies demonstrated the efficacy of boron-containing materials in improving the catalytic activity for hydrogen evolution. It has been discovered that when a boron atom is close to a carbon atom, the valence orbital energy levels of the carbon atom are lowered. Park *et al*. [4] presented The HER activity of B, Mo, Mo_2B, α-MoB, β-MoB, and MoB_2 catalysts. The HER kinetics rise dramatically as the boron concentration rises. The findings demonstrate that boron inclusion had significantly enhanced the molybdenum catalyst.

Jian *et al*. [5] introduce a material of MoO_2 layer on Mo foil, $MoSe_2/MoO_2$ hybrid nanosheets with an abundant edge and high electrical conductivity can be synthesized on the surface of Mo foil to improve HER on the material. The developed MoSe2/MoO2/Mo exhibits highly improved HER performance