Sulfur on molybdenum carbide as an promoter for high efficient hydrogen evolution reaction

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Due to the exergonic hydrogen binding energy property of Mo_2C, weakening the binding energy facilitates HER performance by shifting the HER volcano position toward the top. Here, we hypothesized that the sulfur which is well known as fractious catalyst poison will be an long-lasting adsorbate on Mo_2C and demonstrated the role of sulfur by using the density functional theory calculations. Interestingly, simulation result shows that the intermediate sulfur coverage ($\Theta S=0.50$ or $\Theta S=0.75$) leads an unfavorable hydrogen adsorption which makes energetic penalty resulting in decrease of hydrogen binding energy to reach an almost thermoneutral value. To support this theoretical results we designed sulfur doped Mo_2C without destroying Mo_2C crystal structure sucessfully. And thus synthesized sulfur doped Mo_2C catalysts showed significant enhancement toward hydrogen generation having -91.88mV overpotential to achieve-10mA/cm^2. The doped sulfur contributed to change the hydrogen binding energy by occupying original hydrogen adsorption site leading to unfavorable hydrogen adsorption instead.