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Tuning the Catalytic Properties of Monolayer MoS2 through Doping and Sulfur Vacancies SATVIK LOLLA, State of Maryland, ROSE LUO, National Graphene Research and Development Center — Fuel cells in vehicles cause carbon monoxide, one of the most dangerous gases in the atmosphere. To reduce the amount of CO in the atmosphere, scientists have focused on the adsorption of oxygen. The best substrates used today are platinum and palladium, which are very expensive. One promising cheaper substrate is monolayer MoS2. However, sulfur is a chemically inert site for the oxygen, which greatly decreases the catalytic potential of MoS2 sheets. Therefore, we carried out first-principles calculations to study the effect of substitutional doping and creating sulfur vacancies on the catalytic properties of MoS2. We calculated the adsorption energy of O on doped MoS2 sheets with vacancies, and compared it to the adsorption energy of O on a Pd monolayer. We found that doping MoS2 with Ir, Rh, Co and Fe significantly decreased the adsorption energy, to below 4 eV, indicating that doped MoS2 is a more effective catalyst than Pd. Incorporating sulfur vacancies into the doped MoS2 sheet was extremely effective and decreased the adsorption energy drastically. We concluded that a combination of doping and creating vacancies in monolayer MoS2 sheets can impact the catalytic behavior and make it a more effective catalyst than Pt and Pd.

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