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【655】 Exploring point defects in the 1T' and 2H phases of single-layer MoS₂

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The metastable 1T' polymorph of monolayer Mo and W dichalcogenides has recently been predicted to realize the quantum spin Hall insulator phase. Furthermore, the coexistence of this polymorph with the stable semiconducting 2H phase has been observed. In the 2H phase, point defects have widely been studied, while the effect of defects in the 1T' phase has not been investigated to date. Here, we fill this gap providing a complete picture of point defects in single-layer MoS₂. We consider vacancy, antisite and adatom defects and examine their thermodynamic stability and magnetic properties. We conclude that all considered defects have lower formation energies in 1T'-MoS₂ compared to the semiconducting 2H phase.

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