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Trends in Defect Stability and Electronic Properties of 3d TM-Doped WSe_2

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Dilute magnetic semiconductors (DMSs) offer a promising route to novel hybrid electronic devices that can integrate logic processing, communication, and data storage into a single integrated circuit (IC). These DMS-based hybrid devices can use magnetic or electric force, voltage and light to manipulate electron charge and spin, potentially enabling smaller, faster, and more energy-efficient multifunctional chips.
Two-dimensional (2D) transition metal dichalcogenides (TMDCs) are particularly appealing for DMS applications due to their excellent spin relaxation times and long spin diffusion lengths. Unlike graphene, TMDCs have an adjustable bandgap and exhibit stronger spin-orbit coupling—features that are essential for spin-based logic and non-volatile memory technologies. However, since TMDCs do not naturally possess magnetic properties, it is necessary to induce magnetism through doping.
In this study, we explored the electronic structure and energetic stability of single 3d transition metal (TM) dopants in WSe_2 monolayer using density functional theory (DFT) calculations. Our findings reveal that the chemical stability of TM dopants in WSe_2 varies significantly depending on both the doping site within the lattice and the electronic 'd' character of the transition metal. For dopants ranging from Scandium (Sc) to Cobalt (Co), substitutional doping sites are energetically preferred, showing lower formation energies compared to adatom and interstitial doping. In contrast, from Nickel (Ni) to Zinc (Zn), adatom doping becomes more stable, while substitutional doping is energetically unfavorable. It's also worth noting that monolayer WSe_2 inherently possesses a direct bandgap. We find that doping does not always preserve the direct bandgap. Additionally, incorporating 3d transition metal atoms into WSe2 lattice introduces defect energy levels within the bandgap, with the band gap of WSe2 reduced to between 0.05 eV to 1.0 eV across the 3d series. Furthermore, we find that increasing the dopant concentration lowers the formation energy per atom in WSe2, favouring clustering. These results present important implications to the understanding of properties of transition metal dopants in WSe2, as well as in other dilute magnetic semiconductors where the effect of aggregation of dopants has generally been neglected.

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