Contribution ID: **343** Type: **Poster Presentation**

Chemical Trends in defect stability and electronic properties of 3d transition metal doped WS2

Tuesday, 4 July 2023 16:46 (1 minute)

Dilute magnetic semiconductors (DMSs) offers an alternative pathway towards achieving electronic hybrid devices capable of combining the three critical functionalities of logic, communication and data storage, within a single IC chip. Such DMS hybrid devices can use both voltage and light to simultaneously manipulate both the charge and spin of an electron promising more affordable, compact and faster multifunctional chips with lower power consumption. Two dimensional (2D) transition metal dichalcogenides (TMDCs) have promising magnetic properties suitable for DMS applications due to their superior spin relaxation times and diffusion lengths. In contrast to graphene, TMDCS exhibit a tuneable bandgap and stronger spin-orbit coupling which are a prerequisite for spin logic and non-volatile data storage. However, TMDCs are not intrinsically magnetic, hence, it is important to engineer magnetism in them in order to realize their potential as DMS materials.

In this work, we investigate the energetic stability and electronic properties of 3d transition metal defects in single layer WS2 at different lattice locations, using Density Functional theory electronic structure calculations. We find that the chemical stability of a transition metals in WS2 is strongly dependent on the doping lattice site, and its 'd' character across the 3d series.
Specifically, from Sc to Co, the substitutional site is found to be energetically more favorable with lower formation energies in comparison to the adatomic and interstitial doping. However, from Ni to Zn, the energetic stability shifts towards the adatomic doping location, with the substitutional site becoming highly unfavourable. Even though intrinsic monolayer WS2 has a direct bandgap, we find that doping does not always preserve the direct bandgap. Furthermore, incorporating 3d transition metal atoms into its lattice introduces defect energy levels within the bandgap, with the band gap of doped WS2 increasing by 1.2 eV from Sc to Mn, while narrowing down by 1.3 eV from Mn to Zn. Furthermore, we find that increasing the dopant concentration lowers the formation energy in WS2, favouring clustering. These results present important implications to the understanding of the properties of transition metal dopants in WS2, as well as in other dilute magnetic semiconductors where the effect of aggregation of dopants has generally been neglected.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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Session Classification: Poster Session 1

Track Classification: Track A - Physics of Condensed Matter and Materials