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Defect induced magnetism in transition metal dichalcogenides. MAHTAB KHAN, University of Central Florida — Single layer (SL) transition metal dichalcogenides (TMDCs) (MX_2; M= transition metal such as Mo, W and X = S, Se, Te) have attracted a lot of attention due to their intriguing electronic and optical properties. SL TMDCs are direct band gap semiconductors, which can be used to produce smaller and more energy efficient devices such as transistors and integrated circuits. Moreover, the band gap lies in the visible region, which makes them highly responsive when exposed to visible light, a property with potential applications in optical detection. Despite their success as a fascinating SL semiconductor, magnetism in TMDCs has remained almost unexplored. Due to their technological importance wafer scale production of TMDCs is required. The types of defect observed in TMDCs depends on the fabrication process. The most common experimental techniques used to produce large chunks of SL MoS2 are i) mechanical exfoliation, ii) chemical vapor deposition, and iii) physical vapor deposition. Defects usually play an important role in tailoring electronic, optical and magnetic properties. We performed standard first principle calculations to show that certain defects induce magnetism in TMDCs. In particular we study two types of defects: i) the M vacancy defect and ii) the antisite defect M_X. We find that certain TMDCs exhibit an exceptionally large magnetic moment in the presence of these defects. In addition, we show that the value of their magnetic moment can be tuned by changing the defect density. Our findings considerably improve the understanding of defect induced magnetism in SL TMDCs and should benefit their potential applications in spintronic devices.

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