Defect-induced magnetic coupling in layered $PtSe_2$

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Many Transition-Metal Dichalcogenides (TMDs) have attracted great interest for being exfoliable into atomically thin structures. Certain Noble-Metal Dichalcogenides (NMDs) with chemical formula MX_2 (M=Pt,Pd and X=S,Se,Te), such as $PtSe_2$, take a special place among two-dimensional materials: They can be grown at low temperatures of 450°C by thermally assisted conversion, rendering them compatible with current silicon-based semiconductor technologies.[1] Additionally, NMDs feature strong quantum confinement, including metal-to-semiconductor transitions, high infrared absorption, and high carrier mobilities. Hence, they are some of the most promising candidates for 2D-material based photodetectors, nanoelectromechanical sensors, and chemical sensors.[2] More recently, the occurrence of magnetism in few-layer $PtSe_2$ due to point- and edge-defects has gained a lot of attention.[3–5] Those defects are highly relevant for saturable absorbers, coupling with surfactants, and might interact with the type-II Dirac states present in semi-metallic bulk $PtSe_2$. In this work, we applied Density Functional Theory (DFT) methods, with the aim to study the occurrence, distribution, and coupling of magnetic defects in $PtSe_2$ from a single layer to the bulk material, including vacancies, interstitials, and antisite defects. Engineering the magnetic properties of layered $PtSe_2$ via controlled induction of defects could provide completely new avenues for the design of novel sensors and spintronics.

References

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