Investigating the effect of point defects on the electronic and spintronic properties of $PtSe_2$

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$PtSe_2$ belongs to the group 10 Noble Metal Chalcogenides (NMCs) and has recently attracted notable interest in the scientific community due to its vast range of applications in photonics, optoelectronics, and sensing.[1] Recently, other interesting features of this system were reported, elucidating the effect of different stackings and point defects in electromechanical properties and spintronics properties respectively.[2,3,4] However, several open questions remain, mainly in relation to the impact of point defects' position in electronic structure, and also to the different configurations that result in magnetic ordering in mono- and few-layers of $PtSe_2$. In this current work, we investigate the effect of different positions of Platinum and Selenium vacancies in the band structure of 1 to 4 layers. The formation energy of these defects was also calculated using Density Functional Theory (DFT) methods. Additionally, aberration-corrected STEM observations of liquid-phase exfoliated[5] $PtSe_2$, were conducted using the HAADF detector of NION UltraSTEM operated at 200kV. By comparing and contrasting our theoretical predictions with Z-contrast measurements, we aim to better understand the effect of observed defect configurations on the electronic and spintronic properties.

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