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Effect of hydrogenation on magnetic properties of heavy transition-metal dichalcogenides[1] PRIYANKA MANCHANDA, S. -H. LIOU, AXEL ENDERS, D. J. SELLMYER, RALPH SKOMSKI, University of Nebraska, Lincoln — Two-dimensional transition-metal dichalcogenides (2D TMDs) are emerging as a unique class of materials because of their underlying fundamental physics and technological applications in electronics, sensors, energy storage, photonics, and spintronics. The outstanding electronic properties of 2D TMDs can be further tuned by various external means, such as control of external electric field, chemical functionalization, alloying, and strain. The electronic and magnetic properties of chemical functionalized 2D TMDs is of special interest. Experimentally, adsorbed fluorine has been shown very recently to create a small magnetic moment of 0.06 emu/g in MoS_2 nanosheets. Although several studies as well as review articles on the properties of TMDs have been published in the past few years, Mo and W chalcogenides are most widely studied among the "beyond-graphene" 2D TMDs. However, studies of chemical functionalization on TMDs containing heavy TMDs such as Ta and Pt are still infancy. In the present work, we investigate the effect of hydrogenation on the magnetism of $PtSe_2$ monolayers using density-functional theory. We find that the hydrogen induces a magnetic moment of 0.7 $_B$ per unitcell. This work has been supported by ARO, and DOE-BES.

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