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Electronic and magnetic properties of $NbSe_2$ monolayer doped vacancy and transition metal atoms[1] PRIYANKA MANCHANDA, DAVID SELLMYER, RALPH SKOMSKI, Univ of Nebraska - Lincoln — Two-dimensional transition-metal dichalcogenides (2D TMDs) have attracted much attention recently due to potential applications including optoelectronic devices. Atomically thin layers of materials such as MoS_2, WS_2, NbS_2, $NbSe_2$, $TaTe_2$ can easily be synthesized by exfoliation techniques and exhibit variety electronic phases such as metal, semiconductor, superconductor depending on the choice of metal. Most of the TMDs are nonmagnetic and various techniques have been proposed to induce or modulate magnetic properties that are essential for nanoelectronic device applications. We use DFT calculations to analyze the effect of strain, hydrogen adsorption, and doping. Emphasis is on the magnetic properties of $NbSe_2$ monolayers containing vacancies and $3d$ transition metal atoms. We find that magnetism can be induced by vacancy creation and transition metal-substitution in $NbSe_2$, with effects similar to strain and hydrogen adsorption. The moment mainly arises from the localized nonbonding 3d electrons of the transition-metal atoms. Our findings contribute to the ongoing search "for-better-than-graphene" thin-film materials for novel electronic devices.

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