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Electronic properties of rhenium and niobium doped tungsten disulfide monolayers EDUARDO CRUZ-SILVA, AMBER MCCREARY, ZHONG LIN, NESTOR PEREA-LOPEZ, ANA ELIAS, HUMBERTO TERRONES, MAURICIO TERRONES, Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University — Layered transition metal dichalcogenides (TMDs), have attracted great attention due to their electronic and optical properties. In particular, MoSand WSshow an indirect to direct electronic band gap transition when reduced to a monolayer, and display photoluminescence as a consequence. While there are proposed applications for MoSand WSas electronic and optoelectronic devices, control of their electronic properties needs to be reached before these applications can be scaled. In this sense, chemical doping has been recently shown to allow the modification of the electronic properties of MoSmonolayers by substitution of either transition metals or the chalcogen. Here we present a study of the electronic, magnetic, and chemical properties of doped WSmonolayers by performing *ab initio* calculations. Substitution of tungsten atoms with either niobium or rhenium results in the formation of new states in the vicinity of the Fermi energy that allow to tailor the electronic band gaps, which results in different electronic and optical properties.

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