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Optical and Electronic Properties of doped-MoS2: Joint Theoretical/Experimental Study MILLER EATON, HANSIKA SIRIKUMARA, HASSANA SAMASSEKOU, DIPANJAN MAZUMDAR, THUSHARI JAYASEKERA, Southern Illinois University Carbondale, LAALITHA LIYANAGE, MARCO BUONGIORNO NARDELLI, University of North Texas — Substitutional doping of transition metal dichalcogenides (TMDs) is an attractive way of engineering their electronic properties. The dependence of optoelectronic properties of TMDs on the dopant is largely under-explored. In this work, we will discuss how different species affect the optical properties of MoS2. The electronic structure calculations of doped TMDs are carried out using Density Functional Theory with the recently developed ACBN0 functional, a pseudo-hybrid Hubbard density functional that is a fast, accurate and parameter-free alternative to traditional DFT+U and hybrid exact exchange methods [L.A. Agapito, S. Curtarolo, and M. Buongiorno Nardelli, Phys. Rev. X 5, 011006 (2015)]. We compare our ACBN0 predictions with measurement of the electronic and optical properties of pristine and niobium doped MoS2 films synthesized via physical vapor deposition and characterized using spectroscopic ellipsometry and optical spectroscopy.

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