Abstract Submitted
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Electronic and optical properties of monolayer and few-layer of distorted transition-metal dichalcogenides[1] PIERRE DARANCET, Department of Applied Physics and Applied Mathematics and Department of Physics, Columbia University, ANDREW J. MILLIS, Department of Physics, Columbia University, CHRIS A. MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Groups IV, V, and VI- transition-metal dichalcogenides (TMDC) are layered compounds exhibiting a wealth of competing phenomena, ranging from charge density waves (CDW) to Mott transitions. We present investigations using density functional theory (DFT) and DFT+U regarding the electronic structure and electronic correlations arising in distorted tantalum disulfide (TaS2). We show that the monolayer material is a Mott insulator while the bulk is a metal, in contradiction with much of the existing literature, which argues that the bulk material is a Mott insulator. Properties of the few layer system will also be presented.Finally, we will discuss the influence of these competing energy scales on the transport and optical properties of these materials.

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