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Electronic Structure and Charge-Density Wave Instabilities in Monolayers of Transition Metal Dichalcogenides[1] PIERRE DARANCET, Dept of Applied Physics and Applied Mathematics, Columbia University, ANDREW J. MILLIS, Dept of Physics, Columbia University, CHRIS A. MARIANETTI, Dept of Applied Physics and Applied Mathematics, Columbia University — Transition metal dichalcogenides (TMDC) are layered materials displaying a variety of charge-density wave (CDW) instabilities and complex phase diagrams for group IV & V transition metals. Recent progress in mechanical exfoliation and device fabrication now allow for electrical characterization and gating of individual, 3-atom thick layers [1] of TMDCs, providing new probes of the complex many-body interactions arising in these compounds. In this talk, I will present our investigations using density functional and dynamical mean-field theory regarding the electronic structure and electronic correlations arising in distorted monolayers, bilayers, and trilayers of octahedral group V TMDCs. We will examine the importance of doping, crystal fields, and many-body interactions, and their influence on the transport and optical properties of these materials upon distortion. [1] K. S. Novoselov et al., PNAS 102, 10451 (2005) .

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