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Stacking-dependent electronic structure of TaS₂¹ PIERRE DARANCET, Argonne Natl Lab — Among transition metal dichalcogenides, 1T-TaS₂ is known for its so-called Star of David charge density wave (CDW) conducive to a transition from a high symmetry metal into an odd-electron-number insulator, suggesting a Mott transition. While DFT correctly captures the lattice distortion and the opening of an in-plane gap, it also predicts that interlayer coupling destroys the Mott state leading to the delocalization of electrons out-of-plane [1]. In the past two years, new experimental findings have challenged the DFT description by observing a ground state Mott insulating phase that can be transformed into a long-lived metallic state by light [2], and voltage pulses [3]. Here, we explain these findings using DFT calculations that takes into account the previously theoretically ignored 13-layer periodicity of the CDW. We determine the thermally accessible configurations for the 13-layer-thick unit cell of TaS₂ and compute the electronic structure of these systems as well as the conditions of emergence of an insulating state. [1] Ge and Liu, Phys. Rev. B (2010); Liu, Phys. Rev. B (2009); Darancet et al., Phys. Rev. B (2014); [2] Yu et al., Nat Nano (2015); [3] Tsen et al., PNAS (2015); Vaskivskyi et al., Science Adv. (2015); Cho et al., Nat. Comm. (2015); Ma et al. Nat Comm

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