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Electronic states at transition metal dichalcogenide lateral heterointerfaces[1] OSCAR AVALOS-OVANDO, Ohio University, DIEGO MASTROGIUSEPPE, Instituto de Fisica Rosario, SERGIO ULLOA, Ohio University — Materials with different band gaps are typically used to create heterostructures that enable band sculpting, depending on different shape and boundaries of the systems. These are used in diode lasers and high-speed transistors devices. Potential material candidates for such heterostructures at the monolayer level are the family of transition-metal dichalcogenides, MX_2 (with M=Mo,W and X=S,Se), especially interesting materials with strong spin-orbit coupling and valley degrees of freedom. We consider lateral interfaces between pairs of these materials, and study the effect of different boundary geometries, motivated by recent experimental reports of the growth of such interfaces with different geometries [2,3]. Using an effective 3-orbital tight-binding model [1], we focus our attention on monolayer ribbons and triangular flakes. We analyze the formation of edge/interface states for different gap nesting materials. We study the spatial distribution and orbital character of the wave functions throughout, as well as their dependence on interface termination. [1] G. B. Liu et al., PRB 88, 085433 (2013). [2] C. Huang et al., Nat. Mat. 13, 1096 (2014). [3] Y. Gong et al., Nat. Mat. 13, 1135 (2014).

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