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Interfacial states in 2D lateral heterostructures¹ OSCAR ÁVALOS OVANDO, Ohio University, U.S.A., DIEGO MASTROGIUSEPPE, Instituto de Física Rosario, Argentina, SERGIO ULLOA, Ohio University, U.S.A. — Recent years have seen the birth and manipulation of 2D materials, such as graphene, transition metal dichalcogenides (TMD), silicine and germanene, among others. Heterostructures (HS) between different 2D materials have shown distinct properties with respect to their pristine counterparts [1]. We need to understand the role of these unique atomic interfaces, considering different material features. Here we present our study of the formation of states at the 2D interface between different TMDs. We consider HSs composed of adjacent nanoribbons, which we model via a tight-binding approach with experimental and DFT parameters. We study the effect of different boundary geometries, such as zigzag and armchair, and analyze the formation of edge/interface states for different gap-nesting conditions. We find strongly localized interface states, lying in the band gap as well as in the continuum. Finally, we compare our numerical results with HSs of other hexagonal lattices, such as graphene, silicine or germanene [2], where low-energy states can be described by a Dirac equation with position-dependent mass across the interface. [1] M.-Y. Li et al., Mater. Today 19, 322 (2016). [2] L. Matthes et al., PRB 86, 205409 (2012).

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