

Abstract Submitted
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Symmetry origins of the 'caldera' valence band distortion in 2D semiconductors PENGKE LI, IAN APPELBAUM, Univ of Maryland-College Park, PHYSICS DEPARTMENT TEAM — The electronic structures of many two-dimensional van der Waals semiconductors exhibit various fascinating properties distinct from their three-dimensional bulk counterparts. Through an examination of their lattice symmetries, we identify several universal rules dictating their band dispersion in the monolayer limit, where in-plane mirror symmetry and quantum confinement play critical roles. Taking group-III metal monochalcogenides (such as GaSe) as an example, we reveal the origin of the unusual 'caldera' shape of the valence band edge (otherwise inelegantly dubbed an 'upside down Mexican hat'), which we show is surprisingly common among other 2D semiconductors (such as in phosphorene for k along its zigzag direction). Reference: arXiv:1508.06963

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