Abstract Submitted
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Electronic and thermoelectric properties of Mexican hat bands in van-der-Waals materials[1] DARSHANA WICKRAMARATNE, University of California - Riverside, FERDOWS ZAHID, The University of Hong Kong, Hong Kong SAR, China, ROGER LAKE, University of California - Riverside — Mexican hat dispersions are relatively common in few-layer two-dimensional materials. In one to four monolayers of the group-III chalcogenides (GaS, GaSe, InS, InSe) and Bi_2Se_3 the valence band undergoes a band inversion from a parabolic to an inverted Mexican hat dispersion as the film thickness is reduced from bulk to a single monolayer. The band inversion is robust against changes in stacking order, omission or inclusion of spin-orbit coupling and the choice of functional. The Mexican hat dispersion results in a $1/\sqrt{E}$ singularity in the two-dimensional density of states and a step-function turn on in the density of modes. The largest radius of the ring of states occurs for a single monolayer of each material. The dispersion with the largest radius coincides with the maximum power factor and ZT for a material at room temperature. Ab-initio electronic structure calculations are used with a Landauer approach to calculate the thermoelectric transport coefficients. Analytical models of the Mexican hat and the parabolic dispersions are used for comparison and analysis. Vertically biased bilayer graphene could serve as an experimental test-bed for measuring this effect since the radius of the Mexican hat band edge increases linearly with vertical electric field.

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