Realization of nearly dispersionless bands with strong orbital anisotropy from destructive interference in twisted bilayer MoS_2

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Recently, van der Waals 2D materials stacked with a twist between adjacent layers emerge as rich platforms for the study of various strongly correlated phenomena with high tunability. Here, we use an ab initio based approach to characterize the electronic properties of twisted bilayer MoS2. We report that, in marked contrast to twisted bilayer graphene, slightly hole-doped MoS2 realizes a strongly asymmetric px-py Hubbard model on the honeycomb lattice, with two almost entirely dispersionless bands emerging due to destructive interference. The origin of these dispersionless bands, is similar to that of the flat bands in the prototypical Lieb or Kagome lattices and co-exists with the general band flattening at small twist angle due to the Moire interference. We study the collective behavior of twisted bilayer MoS2 in the presence of interactions, and characterize an array of different magnetic and orbitally-ordered correlated phases, which may be susceptible to quantum fluctuations giving rise to exotic, purely quantum, states of matter.