Ultraflat bands and shear solitons in Moiré patterns of twisted bilayer transition metal dichalcogenides

Manish Jain
Department of Physics
Indian Institute of Sciences
Bangalore 560012

Ultraflat bands in twisted bilayers of two-dimensional materials have a strong potential to host Mott-insulating phases at half-filling. Using first principles density functional theory calculations, we show the emergence of ultraflat bands [1] at the valence band edge in twisted bilayer MoS_2, a prototypical transition metal dichalcogenide. The computed band widths, 5 meV and 15 meV for 56.50 and 3.50 twist angles respectively, are comparable to that of twisted bilayer graphene near 'magic' angles. Large structural transformations in the Moiré patterns lead to the formation of shear solitons at stacking boundaries and strongly influence the electronic structure. We extend our analysis for twisted bilayer MoS_2 to show that flat bands can occur at the valence band edge of twisted bilayer WS_2, MoSe2 and Wse_2 as well.

[1] Mit H. Naik and Manish Jain, arXiv:1803.09240.