Radial Rashba spin-orbit fields in commensurate twisted transition-metal dichalcogenide bilayers

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In commensurate twisted homobilayers, purely radial Rashba spin-orbit fields can emerge due to the interaction of the twisted hidden Rashba spin-orbit coupling (SOC) from each layer [1]. We calculate the band structures and the spin-orbit fields close to the high symmetry points K and Γ of commensurate twisted transition-metal dichalcogenide homobilayers (WSe_2, $NbSe_2$ and 1T-WTe_2) from first principles using density functional theory (DFT) calculations. The observed in-plane DFT spin textures are mostly radial and can in large parts be described by a model Hamiltonian, which consists of two continuum models for the two layers, including SOC terms and interacting by a general (spin-conserving) interlayer coupling. We additionally investigate the effects of an electric field, different lateral shifts and increasing interlayer distance, all three of which can modify the radial Rashba structure.

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References

[1] Frank et al, "Emergence of radial Rashba spin-orbit fields in twisted van der Waals heterostructures", Physical Review B 109, L241403 (2024).

Figures

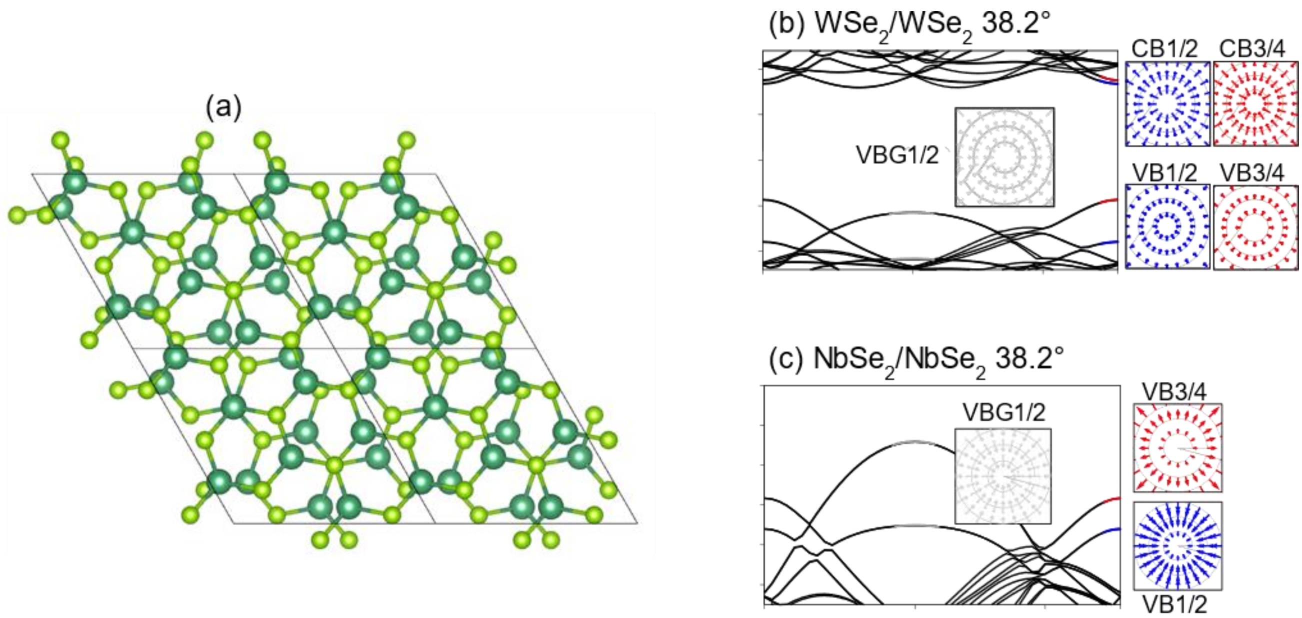

Figure 1: (a) Commensurate twisted (38.2°) $NbSe_2$ bilayer DFT supercell. (b)-(c) Band structure and radial in-plane spin textures (at K and Γ) for twisted WSe_2 (b) and $NbSe_2$ (c) bilayers.