

I. INSTRUCTIONS

Each directory contains the Fourier components of the moiré potential terms appearing in the following Hamiltonian:

$$\tilde{\mathcal{H}}_{K\uparrow} = \begin{pmatrix} -\frac{(\mathbf{p}-\hbar\boldsymbol{\kappa}_b+e\mathbf{A}_b)^2}{2m^*} + h_{\text{kin},b}^{h.o.} + \Delta_b(\mathbf{r}) & \tilde{\Delta}_T(\mathbf{r}, \mathbf{k}) \\ \tilde{\Delta}_T^\dagger(\mathbf{r}, \mathbf{k}) & -\frac{(\mathbf{p}-\hbar\boldsymbol{\kappa}_t+e\mathbf{A}_t)^2}{2m^*} + h_{\text{kin},t}^{h.o.} + \Delta_t(\mathbf{r}) \end{pmatrix}. \quad (1)$$

Here, Δ_b and Δ_t denote the bottom and top-layer potentials, respectively, i.e.

$$\Delta_{b/t}(\mathbf{r}) = \tilde{V}_\varepsilon(\mathbf{r}) \mp \tilde{V}_f(\mathbf{r})/2 + V_{p,b/t}(\mathbf{r}) + V_{s,b/t}(\mathbf{r}). \quad (2)$$

A detailed description of all the above terms can be found in arxiv:2508.17673.

File Descriptions. The meanings of the various data files are summarized as follows:

- `A2` → $A_{b/t}^2$
- `Us` → $V_{s,b/t}$
- `eps` → $V_{\varepsilon,b/t}$
- `Es-band.dat` → DFT band structure data (in units of eV)
- `POSCAR` → Unrelaxed moiré atomic structure
- `CONTCAR` → Relaxed moiré atomic structure
- `CONTCATprim` → Relaxed monolayer TMD atomic structure
- `graph.pb` → Machine-learning force field

Units. The physical units of the quantities are as follows:

- $T_{v,g}$, $T_{cv,g}$, $T_{vc,g}$, $V_{s,b/t,g}$, $V_{f,g}$, $V_{\varepsilon,g}$, and $V_{p,g,b/t}$: meV
- $A_{b/t}^2$ and $A_{b/t,x/y,g}$: atomic Rydberg units
- $B_{u,b/t,g}$: tesla

Data Format. Each `.dat` file contains Fourier components up to the tenth shell. The first and second columns specify the moiré reciprocal lattice vector \mathbf{g} , while the third and fourth columns provide the real and imaginary parts of the corresponding Fourier components.

Model Parameters. The parameters used for the kinetic energy terms and momentum-dependent interlayer tunneling are summarized below.

- **tMoTe₂:**

$$\begin{aligned} E_g &= 1.068 \text{ eV}, & v_F &= 3.527 \times 10^5 \text{ m/s}, & m^* &= 0.63 m_e, \\ \beta_1 &= 2.911 \text{ eV} \cdot \text{\AA}^3, & \beta_2 &= 55.57 \text{ eV} \cdot \text{\AA}^4, & \beta_3 &= -25.38 \text{ eV} \cdot \text{\AA}^5, & \beta_4 &= -319.99 \text{ eV} \cdot \text{\AA}^6. \end{aligned}$$

- **tWSe₂:**

$$\begin{aligned} E_g &= 1.436 \text{ eV}, & v_F &= 5.382 \times 10^5 \text{ m/s}, & m^* &= 0.368 m_e, \\ \beta_1 &= 3.279 \text{ eV} \cdot \text{\AA}^3, & \beta_2 &= 99.94 \text{ eV} \cdot \text{\AA}^4, & \beta_3 &= -30.64 \text{ eV} \cdot \text{\AA}^5, & \beta_4 &= -658.26 \text{ eV} \cdot \text{\AA}^6. \end{aligned}$$