Coulomb-correlated states of moiré excitons and elementary charges on a semiconductor moiré lattice at integer and fractional fillings

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(Dated: August 9, 2022)

Semiconductor moiré heterostructures exhibit rich correlation-induced phenomena at integer and fractional charge fillings with signatures of emergent magnetism, Mott insulating states and generalized Wigner crystals probed by optical spectroscopy of intralayer excitons [1–3]. However, as the staggered band alignment in the underlying WSe2/WS2 heterobilayer system separates photoexcited electrons and holes to form lowest-energy interlayer excitons [4], direct access to interactions among correlated many-body charge states and ground state moiré excitons remained elusive. Here, we use MoSe2/WS2 heterostructures with type-I band alignment [5, 6] to probe Coulomb interactions of elementary charges at integer and fractional filling factors of the periodic moiré lattice with the ground and excited states of moiré excitons [7]. By probing the positive and negative regimes of ambipolar doping, we observe peculiar asymmetry in the response of moiré excitons to electron and hole doping. Moreover, in addition to the formation of positive and negative moiré trions [8–11] reminiscent of their canonical counterparts in monolayer MoSe2 [12], we identify novel many-body states formed between charges at fractional filling factors and moiré excitons. These states exhibit doping-dependent Landé factors as signatures of correlation-induced magnetism [2] at both positive and negative fractional fillings, identifying MoSe2/WS2 heterobilayer as a unique system for studies of correlated phenomena in ambipolar doping regimes.

Van der Waals heterostructures of twisted or lattice-mismatched two-dimensional transition metal dichalcogenides (TMDs) with electron, hole and exciton potentials laterally modulated by moiré effects [13–17] provide a rich platform for optical studies of correlation phenomena arising in flat bands [18, 19] and spatially ordered states [20, 21]. Recent examples of many-body Hubbard physics [16] include the demonstrations of correlation-induced magnetism [2], Mott insulating states [1, 3, 22–26], quantum anomalous Hall effect [27] or Wigner crystals [1, 21] of charges ordered on lattices with integer and fractional fillings [20] and stripes at half-filling factors [28]. In heterobilayers (HBLs), related optical studies have mainly focused on systems with staggered band alignment as in WSe2/WS2 or MoSe2/WS2, characterized by interlayer excitons in lowest-energy states. In the presence of both finite charge doping and photogenerated exciton densities, the signatures in photoluminescence (PL) are thus dominated by moiré trions [8–11] with exciton Landé factors inherited from neutral moiré excitons, implying vanishingly small perturbation of the exciton wave function by the surrounding elementary charges. Signatures of many-body correlations have been detected by probing energy shifts of interlayer exciton transitions of WSe2 and W2 monolayers [1–3, 20, 24], hundreds of meV above the interlayer exciton ground state.

In this work, we use a MoSe2/WS2 heterostructure to establish evidence for novel many-body states formed by ground-state moiré excitons with spatially ordered charges. As opposed to WSe2/WS2 HBLs, the MoSe2/WS2 system has received only little attention in the framework of correlated states in moiré flat bands, and instead raised some controversy regarding its band alignment [5–7, 18, 29–31]. Notably, ab initio calculations predicted a type-II band alignment, with the valence band (VB) maximum located at the K valley of MoSe2 and the conduction band (CB) minimum in the K valley of WS2 below the CB edge of MoSe2 [30]. This, however, was revised in recent work in charge-tunable MoSe2/WS2 heterostructures [5, 6], suggesting type-I band alignment, with the HBL band gap given by that of MoSe2. Our study confirms this band alignment for twisted heterostructures near both high-symmetry configurations of antiparallel (H) and parallel (R) alignment with relative twist angles close to 180° and 0°, respectively. Thus, in both H- and R-type stackings, doping-controlled charges are subject to Coulomb interactions with ground state moiré excitons. With experimental control of both positive and negative doping regimes, we observe a surprising asymmetry in the binding of electrons and holes to moiré excitons, with distinct signatures at integer and fractional fillings of moiré unit cells.
Akin to WSe$_2$/WS$_2$ heterostacks, MoSe$_2$/WS$_2$ HBLs feature relatively large lattice incommensurability of 4%, which inhibits nanoscale and mesoscopic reconstruction ubiquitous in systems with small lattice mismatch as in MoS$_2$/WS$_2$ or MoSe$_2$/WS$_2$ [32–37]. Sizable lattice mismatch stabilizes moiré phenomena by lock HBLs rigidly in the canonical moiré geometry illustrated in Fig. 1a. In this limit, the moiré pattern varies spatially through points of high-symmetry registries with gradual interconversion, giving rise to periodically modulated in-plane moiré potentials for electrons, holes and excitons [13, 16, 17] with distinct, energetically favored spatial positions within the moiré cell as illustrated in Fig. 1a. The superlattice constant of the moiré unit cell depends sensitively on the rotation angle and attains its maximum at about 8 nm [38, 39] in both H- and R-limits. In reciprocal space (schematics in the top panel of Fig. 1b), these two configurations correspond to $K - K'$ and $K - K$ alignments of the MoSe$_2$ and WS$_2$ valleys with twist-angle dependent mini-Brillouin zone (mBz). A key difference between $H$- and $R$-stackings is the ordering of spin-polarized conduction sub-bands of WS$_2$, as illustrated in the bottom panel of Fig. 1b.

To probe the charging behavior of MoSe$_2$/WS$_2$ HBLs at marginal twists near both high-symmetry stackings, we fabricated charge-tunable van der Waals devices illustrated in Fig. 1c. In all devices, the heterostacks were encapsulated in hexagonal boron nitride (hBN) and sandwiched between top and bottom few-layer graphene electrodes. Two devices were assembled from MoSe$_2$ and WS$_2$ monolayers synthesized by chemical vapor deposition (CVD) with triangular shapes facilitating relative orientation, and two more devices were fabricated from monolayers exfoliated from native crystals. From optical alignment of crystallographically terminated crystal edges we aimed at rotational twist angles below 1° in all samples. The dual-gate layout of the field-effect device allows us to subject the MoSe$_2$/WS$_2$ HBL to perpendicular electric field by an imbalanced tuning of the top and bottom gate voltages $V_T$ and $V_B$ as $\Delta V_T = V_T - V_B$ with respect to the grounded reservoir in contact with both MoSe$_2$ and WS$_2$ monolayers, or to vary the doping level by balancing both gates and tuning them simultaneously against the ground as gate voltage $V_G = V_T = V_B$. The former regime probes the static out-of-plane exciton dipole moment via the Stark effect, and the latter allows to shift the Fermi level through the spatially modulated electron and hole potentials of the moiré heterostructure.

We first focus on the charge-neutral regime of moiré excitons in MoSe$_2$/WS$_2$. The top panels of Fig. 2 show cryogenic differential reflection (DR) and PL spectra of $H$-type (Fig. 2a) and $R$-type (Fig. 2b) heterostacks tuned to charge neutrality. In the spectral range between 1.54 and 1.73 eV, the peaks in DR reflect the multiplicity of moiré excitons in twisted MoSe$_2$/WS$_2$ HBLs [5–7]. In the DR spectra of both stackings (top panels), the $M_1$ peak at 1.60 eV, about 30 meV below the transition energy of the fundamental exciton in monolayer MoSe$_2$ at 1.63 eV in our samples, exhibits largest oscillator strength. The consecutive moiré peak $M_2$ is observed at 38 and 35 meV.
FIG. 2. Moiré excitons in charge-neutral MoSe$_2$/WS$_2$ heterostacks. a and b, DR (top panel) and PL (bottom panel) spectra of $H$- and $R$-type heterostacks at charge neutrality with moiré exciton peaks $M_1$, $M_2$ and $M_3$; $M_1$ is the moiré exciton ground state and thus dominates PL due to population relaxation. c and d, Dispersion of DR moiré peaks in perpendicular electric field (proportional to $\Delta V_{TB}$) for $H$- and $R$-type heterostacks, respectively. The dashed lines indicate zero dispersion, signifying marginal interlayer character of the lowest two moiré exciton states $M_1$ and $M_2$. All data were recorded at 3.2 K.

The energetic ordering of moiré exciton peaks detected in DR is consistent with type-I band alignment of both $H$- and $R$-type heterostacks with CB and VB offsets of a few tens and a few hundreds of meV, respectively [5, 6]. The large VB offset manifests pure MoSe$_2$ VB-character for all moiré excitons. The one order of magnitude smaller CB offset in turn implies pure MoSe$_2$ CB-character only for the lowest-energy moiré states $M_1$ and $M_2$, and a hybrid interlayer character for the energetically highest state $M_3$. With this notion, and taking into account that interlayer hybridization favors spin-like bands, the DR spectra in Fig.2a and b are readily explained: the first two moiré states $M_1$ and $M_2$ correspond to the renormalized intralayer exciton of MoSe$_2$ and its first Umklapp peak due to the moiré potential which determines their energy separation by the twist angle with low sensitivity to interlayer coupling. The moiré exciton state $M_3$, in contrast, is formed by VB states of MoSe$_2$ and CB states of WS$_2$ with spin-like character, and the difference in the blueshifts between the respective $M_3$ and $M_1$ peaks is an immediate consequence of the reversed ordering of spin-polarized WS$_2$ sub-bands in $H$- and $R$-type stackings. For ideal $H$- and $R$-type alignments and in the limit of vanishing interlayer coupling illustrated in Fig. 1b, the difference in the blueshifts would be given by $\Delta W_{\text{so}}^2$, the spin-orbit splitting in the CB of WS$_2$. In the DR spectra of Fig.2a and b, the actual difference between of 45 meV between the blueshifts of $M_3$ and $M_1$ moiré peaks implicitly accounts for finite twist and interlayer coupling.

The degree of interlayer character of moiré peaks can be probed experimentally via their dispersion in perpendicular electric field, as obtained from the evolution of the DR spectra with $\Delta V_{TB}$ in Fig. 2c and d for $H$- and $R$-heterostacks. The linear slopes of the moiré peak dispersions would reflect the first-order Stark effect proportional to their out-of-plane electrostatic dipole moment which in turn is a measure of electron delocalization over the two layers with respect to the hole in the MoSe$_2$ layer. In both stackings, $M_1$ and $M_2$ exhibit vanishing dispersions in electric field, confirming their intralayer MoSe$_2$ character. Consistently, the moiré peaks $M_3$ exhibit finite Stark slopes due to their interlayer exciton character.

Having established intralayer character for the ground and first excited moiré exciton states $M_1$ and $M_2$ in both stackings, we focus on their response to charge-carrier doping in Fig. 3. With increasing gate voltages $V_G$, the charging characteristics of PL (Fig. 3a and b) and DR (Fig. 3c and d) exhibit for both stackings transitions from the positive ($p$) through the charge-neutral intrinsic ($i$) to the negative ($n$) doping regimes, reaching on the positive (negative) side into doping levels beyond 1 hole (elec-
electron) per moiré cell. The neutral regime is dominated in both stackings by the ground state peaks $M_1$, accompanied by very weak hot-luminescence from the excited moiré states $M_2$ and another unlabelled feature 20 meV below $M_1$ in the $R$-type sample that vanishes towards charge-neutrality and has no counterpart in the charging diagram of the $H$-stack.

The limits of one hole and electron doping densities per moiré cell are straight-forwardly grasped from the PL charging diagrams of Fig. 3a and b. At highest $p$-doping levels, reached in PL due to non-resonant laser excitation that generates a surplus of holes, the positive trion peak $M_1^+$ emerges at the expense of its neutral counterpart $M_1$, with binding energies of 24 and 35 meV in $H$- and $R$-type stacks. Upon electron doping, $M_1$ converts into the negative trion $M_1^-$ with similar binding energies of 33 and 35 meV in $H$- and $R$-stacks. These positive and negative trions correspond to canonical three-particle complexes with mutual on-site Coulomb interactions, reminiscent of trions in monolayer MoSe$_2$ with nearly identical binding energies [12] in the low-density regimes of Fermi polarons [40]. In both stackings, the hot-luminescence peak $M_2^\pm$ exhibits no obvious signatures on the $p$-doping side, and a weak feature with a small energy shift from $M_2$ upon $n$-doping. Surprisingly, the corresponding feature, labelled as $M_2^\pm$ in Fig. 3c and d, is very prominent in DR throughout the $n$-regime below two electrons per moiré cell, before it converts into $M_2^-$ upon further electron-doping. This transition coincides with the emergence of $M_2^-$ in the $H$-type DR charging diagram in Fig. 3c.

A detailed inspection of the charging behavior in PL and DR reveals a surprising asymmetry in the responses to hole and electron doping. On the hole-doping side, the peak $M_1$ undergoes a transition to $M_1^+$ through consecutive step-like states labelled as $M_1^+$, whereas $M_2$ and $M_3$ disappear abruptly. This charging behavior is reversed on the electron-doping side: the transition from $M_1^- \rightarrow M_1^-$ is abrupt, whereas $M_2$ evolves gradually into $M_2^-$ before jumping abruptly to $M_2^-$. Such contrasting electron and hole charging sequences were observed consistently in all samples of our study with only marginal variations in the energy shifts between charge-dependent features. In the following, we explain these signatures as characteristics of many-body correlated states forming between moiré excitons and charges localized on the lattice of spatially modulated electron and hole potentials.

First, we focus on the limit of 1 charge per moiré cell. The spatially varying electron and hole moiré potentials, $V_e$ and $V_h$, calculated using the continuum model [13] and shown as the two top layers of Fig. 4a for one moiré...
FIG. 4. Interactions of moiré excitons with a charge lattice at integer and fractional fillings. a. From top to bottom: electron and hole potentials $V_e$ and $V_h$ and probability distributions of moiré excitons $M_1$ and $M_2$ with wave functions $\Psi_{1,exc}$ and $\Psi_{2,exc}$ within one moiré unit cell. Minimum-energy electron and hole localization sites are denoted by sites A and B. b. Spatial positions of one exciton (magenta circles) interacting with electrons (blue circles) on the lattice of 25 neighboring moiré cells at mean fractional fillings of up to one charge per cell (note the two inequivalent exciton positions denoted by open and closed circles for even-denominator fractional fillings). c and d, Experimental (blue data) and theoretical (open and closed magenta points) binding energy of the state $M_2^-$ in $H$- and $R$-type heterostacks, respectively, evaluated as its redshift from $M_2$ as a function of electron filling factor.

unit cell, define charge localization sites A and B at the respective potential minima (blue- and red-most spots in the surface plots of Fig. 4a for electrons and holes, respectively). The two lowest moiré exciton states $M_1$ and $M_2$, with probability distributions shown in the two bottom layers of Fig. 4a as obtained from continuum models [16, 17], form two distinct spatially co-localized pairs with electrons and holes: the ground state moiré exciton $M_1$ is co-localized with the electron at site A, whereas the excited moiré state $M_2$ is co-localized with the hole at site B.

These two configurations are reminiscent of canonical negative and positive trions of MoSe$_2$ intralayer excitons, positive and negative charge carriers are confined in monolayer MoSe$_2$ at such low doping levels, and so are both lowest-energy moiré states $M_1$ and $M_2$. Thus, irrespective of stacking type, the binding energy of the negative trion $M_1^-$ in Fig. 3 is comparable with the value in MoSe$_2$ monolayer [12]. On the p-doping side, in contrast, doping levels exceeding 1 hole per moiré cell are required to form the positive trion $M_1^+$ co-localized with the moiré exciton $M_1$, with a binding energy of similar size as in monolayer MoS$_2$. The binding energies of co-localized trions $M_2^\pm$, formed by moiré exciton $M_2$ with the electron on site B, are a factor of two lower in accord with partial delocalization of the moiré exciton wave function between the sites A and B, as illustrated in the bottom layer of Fig. 4.

At doping levels away from integer filling per moiré cell, the common picture of trion formation between one charge and one exciton in MoSe$_2$ monolayer [12] clearly breaks down. The alternative notion of polaron formation between an exciton and a Fermi sea of charges [40] seems also inapplicable given the spatial ordering of electrons and holes by the in-plane moiré potential. Being in this regime, the states labelled $M_1^+$ and $M_2^-$ rather reflect many-body correlated states formed by Coulomb interactions between ordered charge phases and moiré excitons $M_1$ and $M_2$. Consistently, they exhibit signatures of doping-dependent correlation-induced magnetism [2] with enhanced $g$-factors in perpendicular magnetic fields, as will be discussed elsewhere. Interpreting the redshift of $M_2^-$ from the respective $M_2$ moiré peak as the binding energy of the state, we find support for our interpretation from the good agreement between experiment (blue data points) and theory (magenta points) in Fig. 4c and d: as the filling factor (bottom axis in the theory model) is increased from 0 to 1 electrons per moiré cell with increasing gate voltage (top axis of actual experiments), the binding energy varies from zero up to a maximum of 3 and 5 meV in $H$- and $R$-type stacks, respectively, providing an estimate for the energy scale of many-body interactions among intralayer moiré excitons and elementary charges pinned on a moiré lattice.

Our findings identify MoSe$_2$/WS$_2$ HBLs as a unique material platform for studies of correlated physics in both positive and negative doping regimes. Given the rich variety of theoretically predicted phases in related settings [16, 41–45], the specific heterostructure might prove beneficial in experiments by providing contrasting electron and hole moiré potential landscapes or effective masses in relation to the same set of moiré exciton states. Signatures of doping-induced ferromagnetism exhibited by some of the states in our devices provide strong motivation for future experimental and theoretical work on many-body phenomena in MoSe$_2$/WS$_2$ heterostacks.
### METHODS

**Device fabrication:** MLs of MoSe₂ and WS₂ were either mechanically exfoliated from bulk crystals (HQ Graphene) or obtained from in-house CVD synthesis. Thin flakes of hBN were exfoliated from bulk crystals (NIMs). Devices from hBN-encapsulated MoSe₂/WS₂ HBLs were prepared by dry exfoliation-transfer with alignment close to 0° (R-type) and 180° (H-type) by selecting straight crystal edges.

**Optical spectroscopy:** Cryogenic PL and DR spectroscopy was conducted using home-built confocal microscopes in back-scattering geometry. The samples were loaded into a closed-cycle cryostat (attocube systems, attoDRY1000) with a base temperature of 4 K or a dilution refrigerator (Leiden Cryogenics) operated at 4 K. Both cryogenic systems were equipped with a superconducting magnet providing magnetic fields of up to ±9 T in Faraday configuration. Piezo-stepping and scanning units (attocube systems, ANPxxyz and ANSxy100) were used for sample positioning with respect to a low-temperature apochromatic objective (attocube systems). A wavelength-tunable Ti:Sapphire laser (Coherent, Mira) in continuous-wave mode and laser diodes were used to excite PL. For DR measurements, a stabilized Tungsten-Halogen lamp (Thorlabs, SLS201L) and supercontinuum lasers (NKT Photonics, SuperK Extreme and SuperK Varia) were used as broadband light sources. The PL or reflection signal were spectrally dispersed by monochromators (Roper Scientific, Acton SP2500 or Acton SpectraPro 300i with a 300 grooves/mm grating) and detected by liquid nitrogen or Peltier cooled charge-coupled devices (Roper Scientific, Spec-10:100BR or Andor, iDus 416). A set of linear polarizers (Thorlabs, LPVIS), half- and quarter-waveplates (B. Halle, 310 – 1100 nm achromatic) mounted on piezo-rotators (attocube systems, ANR240) were used to control the polarization in excitation and detection. The DR spectra were obtained by normalizing the reflected spectra to the HBL region (R) to that from the sample region without MoSe₂ and WS₂ layers (R₀) as DR = (R – R₀)/R₀.

**Electron and hole moiré potentials and moiré exciton wave functions:** The two lowest moiré exciton states in type-I MoSe₂/WS₂ HBLs of H- and R-type can be considered as intralayer moiré states in the MoSe₂ layer. To illustrate the probability distribution for the moiré exciton states M₁ and M₂ shown in the two bottom panels of Fig. 4a, we assume that the electron and hole potential landscapes vary periodically [13, 16, 17]:

\[
\Delta_q = \sum_{j=1}^{6} V_j^{(q)} \exp(i b_j \mathbf{r}),
\]

where \( q = e, h; b_j \) are the first-star reciprocal lattice vectors of the moiré pattern, and:

\[
V_{1,2,3}^{(q)} = V_{2,4,6}^{(q)} = V_q \exp(i \psi_q).
\]

Taking into account that the exciton binding energy is much larger than the potential amplitudes \( V_e \) and \( V_h \), we approximate the potential modulation for the exciton center-of-mass as:

\[
\Delta_{exc} = \Delta_e + \Delta_h.
\]

Within this framework we calculate the wave functions of moiré excitons with the following parameters: \( (V_e, \psi_e) = (14 \text{ meV}, 40^\circ) \) and \( (V_h, \psi_h) = (7 \text{ meV}, -40^\circ) \), the moiré superlattice constant is 8 nm and the exciton mass is 1.44 m₀. Using these parameters we plot Fig. 4a, illustrating that the lowest-energy moiré exciton state \( M_1 \) is localized at the minimum of the electron potential, whereas the second moiré exciton \( M_2 \) is mainly localized at the minimum of the hole potential.

**Coulomb-interaction energies:** To calculate the interaction energy (binding energy) of moiré excitons with electrons/holes ordered on a lattice we assume that the exciton is confined in one moiré cell and interacts with surrounding electrons/holes on a lattice as illustrated in Fig. 4b. For each fractional filling we consider a lattice of elementary point charges with different spatially ordered patterns. Due to the lattice symmetry at a given fractional filling, distinct inequivalent positions of excitons are to be considered (empty and filled circles in Fig. 4b) for 1/4, 1/2, and 3/4 fillings.

We further assume that the main contribution to the binding energy stems from charge-induced modification of the electron-hole relative motion \( \rho \equiv (\rho, \theta) = \mathbf{r}_e - \mathbf{r}_h \), where \( \mathbf{r}_e(h) \) are the coordinates of the electron and hole forming the exciton. The corresponding Schrödinger equation takes the form:

\[
-\frac{\hbar^2}{2\mu} \Delta \varphi(\rho) + [V_{K}(\rho) + V(\rho)]\varphi(\rho) = E_{tr}\varphi(\rho),
\]

where \( E_{tr} \) is the exciton energy, \( \mu = m_em_h/(m_e + m_h) \) is the reduced exciton mass, \( m_e \) and \( m_h \) are the electron and hole effective masses, and the Rytova–Keldysh potential [46, 47] of the electron-hole attraction is given by:

\[
V_{K}(\rho) = -\frac{\pi e^2}{2\varepsilon \rho_0} \left[ H_0 \left( \frac{\rho_0}{\rho} \right) - Y_0 \left( \frac{\rho_0}{\rho} \right) \right].
\]

Here, \( e \) is the electron charge, \( \rho_0 \) is the screening length, \( \varepsilon \) is the effective dielectric constant, and \( H_0(x) \) and \( Y_0(x) \) are Struve and Neumann functions.

The interaction of the exciton with the charge lattice is described by the Coulomb sum:

\[
V(\rho) = \pm \frac{e^2}{\varepsilon} \sum \frac{1}{|\beta_e \rho + \mathbf{n}|} - \frac{1}{|\beta_h \rho - \mathbf{n}|},
\]

where the plus and minus signs correspond to positive and negative elementary charges, \( \beta_e = m_e/(m_e + m_h) \), \( \beta_h = m_h/(m_e + m_h) \), and \( \mathbf{n} \) are the coordinates of electrons/holes on the lattice. The two terms in the brackets
The trial function is:

\[ E_B = E_X - E_{tr}. \]

To calculate \( E_X \), we set \( V(\rho) = 0 \), and use in the calculations of both \( E_X \) and \( E_{tr} \) 2D hydrogen-like wave functions with the Bohr radius as variational parameter [48–50] and the basis of six functions [51] with quantum numbers \((n, l) = (1, 0), (2, 0), (2, \pm 1), (4, \pm 3)\) to take into account polarization effects on the exciton relative motion. Due to the lower rotational symmetry of the potential \( V(\rho) \), we also include hydrogen-like wave functions with angular momenta \( l = \pm 1, \pm 3 \). The explicit expression for the trial function is:

\[ \varphi(\rho, \theta) = e^{-\rho \rho} + \zeta e^{-\rho \rho} + \eta e^{-\gamma \rho} \cos \theta + \xi e^{-\delta \rho} \cos \theta. \]

We solve the minimization problem numerically for seven parameters \((\alpha, \beta, \gamma, \delta, \zeta, \eta, \xi)\) using MATLAB R2017B and experimental material parameters of MoSe\(_2\) monolayers [52]: \( m_\alpha = 0.84 m_0 \), \( m_\delta = 0.6 m_0 \), \( \varepsilon = 4.4 \), \( \rho_0 = 0.89 \) nm. The only fitting parameter for comparison between experimental data and theoretical model results is the moiré superlattice constant. In the main text we fit the data with 7 and 6 nm for \( H-\) and \( R-\)type MoSe\(_2\)/WS\(_2\) HBLs, respectively, corresponding to 178.6° and 2.2° twist angles.

Acknowledgements:
This research was funded by the European Research Council (ERC) under the Grant Agreement No. 772195 as well as the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within the Priority Programme SPP 2244 2DMP and the Germany’s Excellence Strategy EXC-2111-390814868. B.P. acknowledges funding by IMPRS-QST. I.B. acknowledges support from the Alexander von Humboldt Foundation. X.H. and A.S.B. developed theoretical models and performed numerical calculations. A.S.B. developed theoretical models and performed numerical calculations. A.H. analyzed the data and wrote the manuscript. B.P. and J.S. contributed equally to this work.

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Data availability: The data that support the findings of this study are available from the corresponding authors upon reasonable request.

Code availability: The codes that support the findings of this study are available from the corresponding authors upon reasonable request.

Competing interests:
The authors declare no competing interests.

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