

Electric-Field Control of Interlayer Binding and Friction in *h*-BN Contacts

Penghua Ying^{1,2}, Michael Urbakh^{2,*} and Oded Hod²

¹*Laboratory for Multiscale Mechanics and Medical Science, SV LAB, School of Aerospace, Xi'an Jiaotong University, Xi'an 710049, China*

²*Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel*



(Received 11 January 2026; accepted 13 May 2026; published 10 July 2026)

Recent studies of two-dimensional layered materials under external electric fields have gained significant attention, as such fields offer a powerful, noninvasive approach to actively modulate surface interactions at the molecular level, enabling real-time and reversible tuning of material properties. In this article, we use fully atomistic molecular dynamics simulations based on machine-learning potentials to predict the dependence of chemifrication on external electric fields in defected layered contacts. By controlling the rate of polar bond formation and rupture, friction can be either increased or decreased depending on the field strength and direction. To extend these atomistic insights to the experimentally relevant low-velocity regime, we develop a physically motivated stochastic model that bridges atomic-scale mechanisms with macroscopic friction behavior. Although demonstrated for hexagonal boron nitride junctions, the proposed mechanism of electrotunable chemifrication is expected to be general and applicable to a broad range of layered materials with polar interlayer bonding.

DOI: [10.1103/s32x-hjrx](https://doi.org/10.1103/s32x-hjrx)

Subject Areas: Materials Science

I. INTRODUCTION

Two-dimensional (2D) layered materials exhibit exceptional physical properties and offer tremendous technological potential in diverse fields, including electronics [1,2], optics [3], mechanics [4,5], and tribology [6–9]. Over the past decade, there has been growing interest in exploring how external electric fields (EFs) influence the properties and performance of these materials [10–12]. This interest is driven by two main factors. First, the rapid transition from internal combustion engines to electric vehicles has created an urgent need for advanced materials that can simultaneously address tribological, electrical, and thermal challenges [13]. In this respect, 2D layered materials, with their multifunctional properties, represent a promising solution, but their operation under high EFs remains poorly understood. Second, applying an external EF provides a powerful, noninvasive means to actively modulate surface interactions at the molecular level [14–16]. This enables real-time, reversible tuning of material properties, opening new opportunities for adaptive and energy-efficient technologies [17]. Notably, practical

applications typically involve large-scale interfaces that inevitably contain structural defects, such as atomic vacancies, steps, edges, and grain boundaries [18–21]. These defects give rise to complex reactive dynamics, making it particularly challenging, but also essential, to understand how electric fields affect the properties of defected 2D material surfaces.

In this article, we demonstrate that applying an external EF enables controlled tuning of the energetics and kinetics of electrically polar bond-pair formation and rupture at contacting defected hexagonal boron nitride (*h*-BN) surfaces. This tunability gives rise to a pronounced modulation of friction at twisted *h*-BN interfaces, where the friction can either increase or decrease depending on the field strength and direction. To this end, we consider *h*-BN bilayers composed of a pristine bottom layer and a top layer containing trivacancies, which enable the formation and rupture of polar bond pairs. To capture the shear-induced dynamics, we develop graph-neural-network- (GNN) based machine-learning potentials (MLPs) trained against density-functional-theory (DFT) reference data. These MLPs accurately reproduce the EF-dependent transition energy barriers (TEBs) for interlayer bond formation and rupture, as well as nonbonded sliding potential energy surfaces (PESs). Using this framework, we perform reactive molecular dynamics (MD) simulations that describe interlayer bonding dynamics and quantify EF effects on both the physical and the chemical contributions to friction with first-principles accuracy. To that end, we decompose the

*Contact author: urbakh@tauex.tau.ac.il

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

total frictional stress into two components [22,23]: *physifrication*, which arises primarily from interlayer Pauli repulsion and elasticity effects, and *chemifrication*, which originates from covalent interfacial bonding. Building on these atomistic insights, we further construct a stochastic phenomenological model to extend our predictions to experimentally relevant low-velocity regimes, thereby bridging between the atomic-scale mechanisms and macroscopic friction behaviors.

II. DFT CALCULATIONS

To investigate the influence of the external EF on interfacial binding and sliding in *h*-BN contacts, we examine two antiparallely stacked bilayer systems: a pristine interface model, with no defects on both contacting layers (V_0V_0), and a defected interface model, where a pristine layer is in contact with a defected *h*-BN layer that incorporates a trivacancy, where two boron and one nitrogen atoms are removed [V_0V_3 ; see Fig. 1(a)]. The latter defected structure, which has been experimentally observed [24,25], exhibits the lowest interlayer bond formation barrier and strongest EF response among all neutral vacancy configurations considered (see Supplemental

Material [26] Sec. 1). All DFT calculations were performed using the projector-augmented-wave (PAW) method [31] with the PBE exchange-correlation density functional approximation [48] and D3(BJ) dispersion corrections [32] as implemented in the VASP package [28,29] (Supplemental Material [26] Sec. 2). EFs of -2 , -1 , 0 , 1 , and 2 V/nm were applied, where positive values defined as fields directed from the bottom (pristine) to the top (pristine or defected) layer.

For the pristine V_0V_0 bilayers, both binding energies and sliding PESs are unaffected by the applied EF (Supplemental Material [26] Fig. S12). This invariance arises from the nonpolar nature of the centrosymmetric antiparallely stacked bilayer, and the rapid decay of the EF induced by the partial charges on the B and N atoms in the infinite hexagonal array into vacuum [50]. In contrast, the defected V_0V_3 bilayers exhibit pronounced EF sensitivity, with both the binding energies and sliding potential energy barrier heights strongly influenced by the field. Using the climbing-image nudged-elastic-band method [27] with 16 images, we identified three distinct interlayer binding states: (i) a single $B_1 - N_2$ bond, (ii) simultaneous $B_1 - N_2$ and $N_1 - B_2$ bonds [marked as 1B and 2B in Fig. 1(d)], and (iii) dual $N_1 - B_2$ bonds [Supplemental Material [26] Sec. 1], where

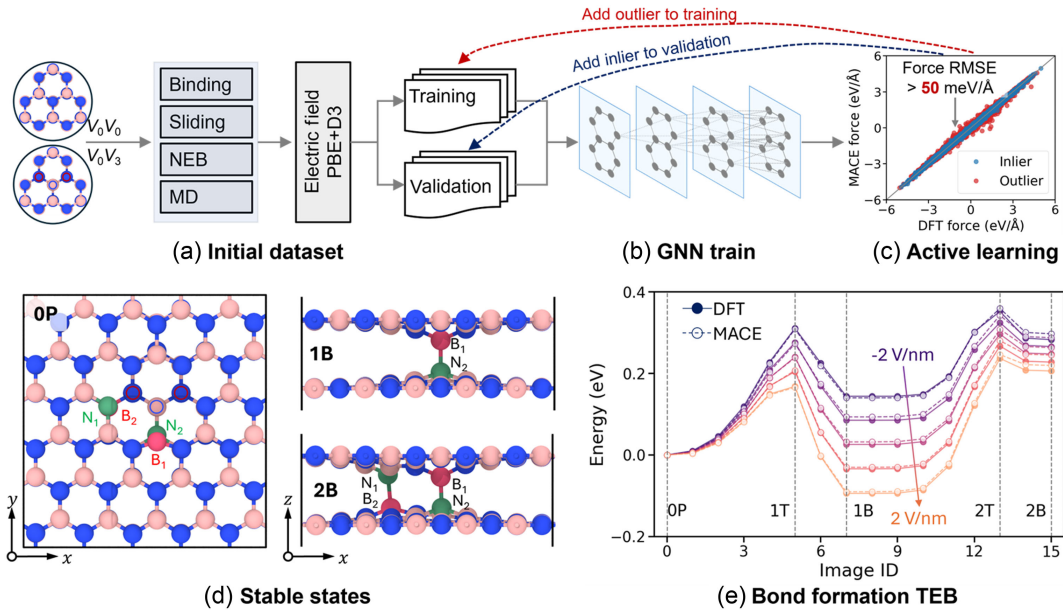


FIG. 1. (a)–(c) Workflow for constructing EF-specific MACE models. (a) The initial dataset includes structures of both pristine (V_0V_0) and defected (V_0V_3) bilayer *h*-BN obtained using MD simulations performed with the foundation MACE model (see Supplemental Material [26] Sec. III), NEB calculations using DFT (see Supplemental Material [26] Sec. I and 2), and manual manipulations of the interlayer distance (binding) and shear (sliding). (b) Schematic illustration of the message-passing algorithm in the GNN potential. (c) Active-learning scheme: structures with force RMSEs > 50 meV/Å (outliers) that emerge from the sliding dynamics of the V_0V_3 model system are added to the training set in the next training iteration, while the remaining structures (inliers) are assigned to the validation set. (d) Snapshots of three stable states: left, initial state (0P, top view); right, one-bond (1B, front view), and two-bond (2B, front view) states. (e) Reaction path for bond formation in the V_0V_3 bilayer system obtained using NEB calculations, as predicted by DFT (open circles) and MACE (filled circles) under various EFs. In panels (a) and (d), atomistic snapshots were visualized using the OVITO package [49], with boron and nitrogen atoms represented by pink and blue spheres, respectively, whereas boron and nitrogen vacancies are indicated by red and blue open circles. In panel (d), the boron and nitrogen atoms involved in the interlayer binding are highlighted by red (B) and green (N).

the subscripts 1 and 2 denote atoms in the top and bottom layers, respectively. All three configurations are stable; however, the third state exhibits a high TEB of 1.45 eV for bond formation and a low barrier of 0.044 eV for bond rupture (Supplemental Material [26] Fig. S2), making it thermally inaccessible at room temperature, with a very short bond lifetime. Consequently, it was excluded from further analysis. Figure 1(e) illustrates the reaction pathway connecting the pristine (0P) state to the one-bond 1B state (via the first transition state “1T” associated with $B_1 - N_2$ bond formation), and subsequently to the two-bond “2B” state (via the second transition state “2T” associated with $N_1 - B_2$ bond formation). The calculated zero-field bond formation and rupture barriers for the $0P \rightarrow 1B$ transition (0.24 and 0.21 eV, respectively) are in good agreement with previously reported DFT values (0.34 and 0.29 eV) [51], with the remaining deviations attributed to differences in the exchange-correlation density functional approximation used (PBE0-TC-LRC + D3 [52] versus PBE + D3 in the present study).

The energy landscape along the reaction pathway exhibits a pronounced dependence on the applied EF, with the TEBs for bond formation and rupture varying approximately linearly with EF strength. The $0P \rightarrow 1B$ formation barrier decreases with EF, at a slope of -0.036 eV/(V/nm), whereas the $1B \rightarrow 2B$ formation

barrier increases with EF, at a slope of 0.031 eV/(V/nm) [see Fig. 2(a)]. The corresponding rupture barriers display opposite trends: The $1B \rightarrow 0P$ barrier increases at a rate of 0.024 eV/(V/nm), whereas the $2B \rightarrow 1B$ barrier decreases at a rate of -0.010 eV/(V/nm) [see Fig. 2(b)]. This EF sensitivity originates from the polar (and polarizable) eclipsed atomic pairs ($B_1 - N_2$ and $N_1 - B_2$), which form oppositely oriented dipoles perpendicular to the contacting surfaces. Under a positive EF, the dipole associated with the $B_1 - N_2$ bond aligns with the field, and thus the bond formation TEB is lowered, whereas the $N_1 - B_2$ dipole opposes the field, which leads to an increased bond formation barrier.

III. EF-SPECIFIC MACHINE-LEARNED POTENTIALS

Capturing stochastic bonding dynamics and frictional behavior during sliding requires reactive MD simulations. Although *ab initio* MD provides accurate interatomic forces derived directly from DFT, its prohibitive computational cost limits the model system dimensions and simulation time-scales that can be addressed. Over the past two decades, MLPs [34,53–55] have emerged as a promising alternative, enabling near first-principles accuracy at a fraction of the computational cost. These approaches efficiently map *ab initio* data onto interatomic forces using linear regression [56,57], kernel-based methods [58,59], and neural networks [60,61], combined with invariant [62] and equivariant [33,63] descriptors to achieve robust and transferable representations.

Building on our previously developed active-learning strategy implemented with a GNN framework, which achieved *ab initio* accuracy in describing binding and friction in defected graphene bilayers [22,23], we extend this approach here to *h*-BN bilayers. Specifically, we use the MACE framework [33] to construct a suite of field-specific MLPs, each trained for a particular EF strength (-2 , -1 , 0 , 1 , and 2 V/nm) against self-consistent DFT reference data, following the active-learning workflow illustrated in Fig. 1(a), thus accounting for field-induced charge redistribution and polarization effects. MACE delivers state-of-the-art accuracy [34,35] through its equivariant message-passing neural-network architecture, which is essential for capturing both physifrication and chemifrication behavior at sliding van der Waals (vdW) interfaces. To encode EF effects, we deliberately break the inversion symmetry typically preserved in potential models [64]. To that end, atoms are explicitly labeled according to their layer (B_1 and N_1 for the top layer, B_2 and N_2 for the bottom layer), enabling distinct treatment of directional interactions (e.g., $B_1 - N_2$ vs $B_2 - N_1$) and thereby incorporating the field-induced asymmetry directly into the model.

After two active-learning iterations [Fig. 1(a); see Supplemental Material [26] Sec. 3 for details], the resulting MACE models achieve energy root-mean-square errors

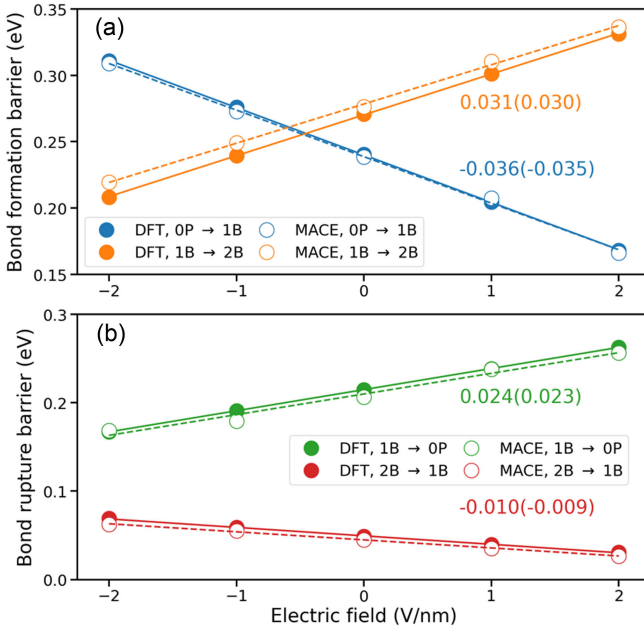


FIG. 2. EF dependence of the TEBs for (a) bond formation and (b) rupture in the V_0V_3 bilayer system along the reaction path shown in Fig. 1(e). Filled circles denote DFT results and open circles are MACE predictions. Blue and orange circles in panel (a) correspond to bond formation barriers for the $0P \rightarrow 1B$ and $1B \rightarrow 2B$ transitions, respectively. Green and red circles in panel (b) correspond to bond rupture barriers for the $1B \rightarrow 0P$ and $2B \rightarrow 1B$ transitions, respectively. Linear slopes of the barrier heights versus EF are reported for DFT and MACE (in brackets).

(RMSEs) < 0.4 meV/atom and force RMSEs < 12 meV/Å across training, validation, and test sets for all EFs (Supplemental Material [26] Fig. S10). Beyond RMSEs, the models reproduce the binding energy curves and the shallow sliding PESs of V_0V_0 bilayers with errors less than 0.2 meV/atom (Supplemental Material [26] Figs. S11 and S12). For the V_0V_3 bilayer, the models accurately capture EF-dependent reaction paths and barriers for interlayer bond formation and rupture [Figs. 1(d) and 2; Supplemental Material [26] Fig. S13]. Together, these results show that the EF-specific MACE models simultaneously resolve weaker vdW interactions (approximately 0.1–1 meV) and stronger covalent bonding (approximately 0.1–1 eV), under applied fields, demonstrating first-principles accuracy over several orders of magnitude. We note that the proposed scheme is of general nature and can be applied to other material interfaces and to different field strengths.

IV. SLIDING DYNAMICS SIMULATIONS

The constructed MACE models enable MD simulations of EF-dependent reactive sliding in pristine (V_0V_0) and defected (V_0V_3) bilayers, in both the aligned and twisted-stacking configurations. In the defected model systems, a surface defect concentration of approximately 1% was considered, which falls within the experimentally relevant range [65,66]. All simulations were performed using the LAMMPS code [67] at room temperature (300 K), under varying EFs (ϵ) and normal loads (σ). In the simulations, the top layer was laterally driven along the zigzag direction by a rigid slider (replicating the top h -BN layer) through a harmonic spring of 0.2 N/m/atom, whereas atoms on the bottom layer were anchored to their initial positions using harmonic springs (0.2 N/m/atom in the x - y plane and 1.0 N/m/atom along the z direction), mimicking a substrate of approximately three layers in thickness (see Supplemental Material [26] Sec. IV for details). Unless stated otherwise, a constant sliding velocity of $v = 10$ m/s was applied. Kinetic friction was averaged over three independent trajectories with different random seeds of the atomic velocities at finite temperature to account for stochastic dynamical effects. We note that at the high-velocity regime dictated by the limitations of the MD simulations, high normal loads in the range of a few GPa (still accessible by tribological experiments [68,69]) were applied to accelerate bond formation kinetics. Extrapolation to lower normal loads and sliding velocities is performed using the stochastic model described below.

We first examine twisted V_0V_3 bilayers, where incommensurate stacking suppresses physifrication [22,23], due to effective cancellation of lateral forces, allowing the EF-dependent chemifrication to be isolated (see Supplemental Material [26] Fig. S26). The top layer is rotated by 9.43° relative to the bottom layer and contains trivacancies [two B atoms and one N atom; see Fig. 3(a)]. This twist angle was chosen to generate laterally periodic supercells that

enable efficient computations, while avoiding interactions between replicated defects [23]. At zero normal load, the activation barrier of approximately 0.2 eV [Fig. 1(e)] yields a typical bond-formation time of $\tau_{\text{bond}} \approx 5$ ns [see Eq. (4)], which is an order of magnitude longer than our total simulation window of approximately 0.5 ns, supporting the fact that we observe no bonding under these conditions. At a low normal load of 2.5 GPa and an EF of 2 V/nm, the barrier reduces to approximately 0.1 eV, and the timescale for bond formation becomes $\tau_{\text{bond}} \approx 100$ ps. Since this is shorter than our total simulation window of 500 ps, bond formation and rupture events, with stick-slip behavior, are clearly observable in the MD trajectories [see Figs. 3(b) and 3(e) and Supplemental Material [26] Video 1]. In contrast, zero and negative fields (0, -2 V/nm) yield smooth, near-zero frictional stress traces, indicating the absence of interlayer bond formation across all trajectories. At a moderate load of 5.0 GPa, bond-induced stress fluctuations emerge under EFs of 0 and $+2$ V/nm, whereas an EF of -2 V/nm shows smooth traces with no interlayer bonding [see Figs. 3(c) and 3(f), and Supplemental Material [26] Video 2]. At a high load of 7.5 GPa, pronounced stick-slip behavior is demonstrated under all EFs considered, reflecting repeating bond formation and rupture events [see Figs. 3(d) and 3(g), and Supplemental Material [26] Video 3]. Specifically, under a field of 2 V/nm, the bond formation barrier reduces to approximately 0.04 eV, and τ_{bond} drops to 5 ps. At this point, the bond formation time becomes smaller than $\tau_{\text{slide}} (= a/v \approx 25$ ps for a lattice spacing $a \approx 0.25$ nm); hence, the bonding saturation behavior that we observe [see Fig. 3(g)].

Similar interlayer bonding dynamics are also observed in aligned V_0V_3 bilayers [see Supplemental Material [26] Sec. VII, Videos 4–6], where the bonding probability is higher due to the greater likelihood of encountering reactive sites in eclipsed configurations. However, in this alignment, friction is primarily governed by Pauli repulsions between the contacting surfaces, rendering the contribution of bonding effects to kinetic friction minor.

As a consistency test, we use Kramers's theory [70] to estimate the peak force from the NEB profiles [Fig. 2(b)] as follows: $F_{\text{rupture}} \approx E_u/x^*$, where $E_u \approx 0.21$ eV is the bond rupture barrier at zero field, and $x^* \approx 0.026$ nm is the typical elongation at which the bond breaks. Dividing this force by the lateral contact area of our supercell [$S \approx 8$ nm²; see Supplemental Material [26] Sec. 4], the resulting lateral stress is approximately 0.16 GPa, in agreement with the stress values of 0.15–0.25 GPa obtained in our MD simulations [Figs. 3(b)–3(d)].

Previous studies have shown that the probability of interlayer bond formation generally increases with normal load, reflecting load-induced TEB reduction (see Supplemental Material [26] Fig. S19) [23,41,71,72]. Here, we find that applying external EFs introduces an additional control parameter, allowing to shift the load

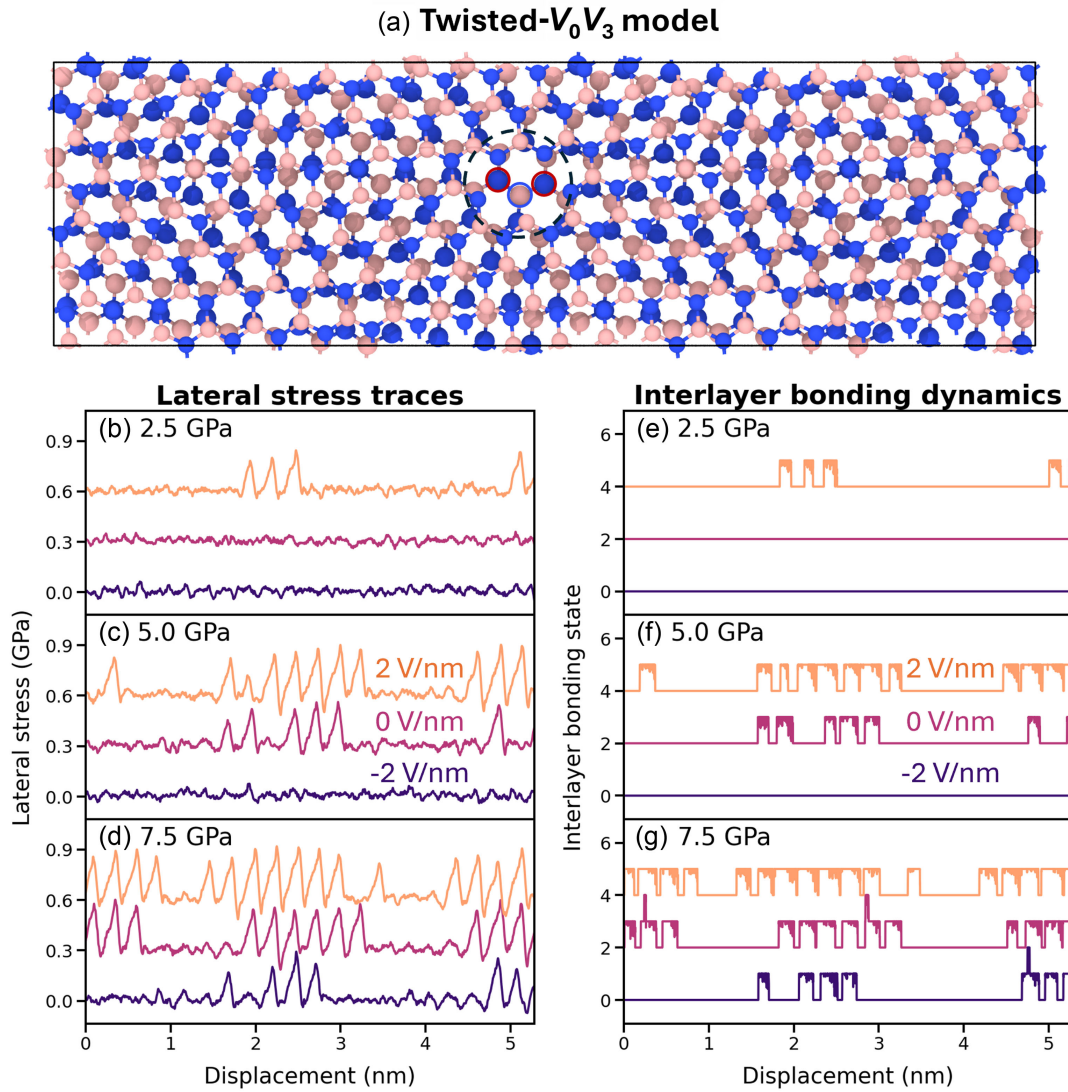


FIG. 3. (a) Top view of the 9.43° twisted V_0V_3 h -BN bilayer with a surface defect concentration of approximately 1%. Boron and nitrogen atoms are represented by pink and blue spheres, respectively. Two boron vacancies and one nitrogen vacancy are marked by red and blue open circles (highlighted with a dashed circle). (b)–(d) Representative frictional stress traces for the twisted V_0V_3 h -BN bilayer obtained from the MLP sliding dynamics simulations at 300 K and a sliding velocity of 10 m/s, under normal stresses of (a) 2.5 GPa, (b) 5.0 GPa, and (c) 7.5 GPa. Each panel compares results obtained under EFs of -2 V/nm (deep purple), 0 V/nm (purple), and 2 V/nm (orange). (e)–(g) Corresponding evolution of the number of interlayer bonds under the same conditions as in (a)–(c). For clarity of presentation, frictional stress curves are vertically offset by 0.3 GPa between adjacent EF traces, while the interlayer bond number curves are shifted upward by two units. Frictional stress data are smoothened using a Savitzky-Golay filter [46] with a window length of 101 and a third-order polynomial, as implemented in the SCIPY library [47].

threshold for bond formation from approximately 3.75 GPa at zero field to approximately 2.5 GPa and to approximately 7.5 GPa at ± 2 V/nm, respectively [Figs. 2(a), 3(e) and 3(g) and Supplemental Material [26] Fig. S17]. Under a load of 7.5 GPa, two-bond formation occasionally occurs under EFs of -2 and 0 V/nm but is absent under $+2$ V/nm [Fig. 3(g)], confirming that positive EFs suppress the occurrence of a second binding event before single-bond rupture [Fig. 2(b) and Supplemental Material [26] Fig. S21]. Since the energy barrier for a single interlayer bond formation (approximately 0.2 eV) is considerably

lower than the typical intralayer h -BN lattice bond energy (approximately 7 eV, [73]), interlayer binding is expected to be fully reversible under shear without causing permanent wear.

V. STOCHASTIC MODEL OF INTERLAYER BONDING DYNAMICS

A key limitation of reactive sliding molecular dynamics simulations is the computational burden involved, which restricts the overall simulation time to the nanosecond

regime. Considering the typical nanoscale dimensions of relevant layered material contacts, this enforces sliding velocities in the range of 1 to 10 meters per second, orders of magnitude higher than experimentally accessible velocities [74]. To bridge this gap, we develop a two-state stochastic model based on the knowledge gained by our atomistic simulation, enabling prediction of interlayer bonding dynamics and its effect on frictional response across a broad range of sliding velocities. The model is based on the following assumptions: (i) transitions between the bound and unbound states follow Arrhenius-type thermally activated kinetics, (ii) transition energy barriers are linearly modulated by external normal loads and EFs, (iii) bond rupture is stress assisted, with the barrier height decreasing linearly with lateral bond extension, and (iv) the bond formation barrier is independent of the interlayer stacking mode.

In this model, the shear-induced transitions between bound and unbound states are described in terms of the survival probability density $p_b(x; \sigma, \epsilon)$, which represents the probability that a bond remains intact at a lateral bond extension between x and $x + dx$, for a given sliding velocity v , normal load σ , and external EF ϵ . The survival probability density evolves according to the following first-order rate equation:

$$\frac{\partial p_b(x(t); \sigma, \epsilon, v)}{\partial t} = \frac{\partial p_b(x; \sigma, \epsilon, v)}{\partial x} v = -k_{\text{off}}(x; \sigma, \epsilon) p_b(x; \sigma, \epsilon). \quad (1)$$

where $k_{\text{off}}(x; \sigma, \epsilon)$ is the bond rupture rate. Since newly formed bonds (at $x = 0$) originate from the unbound state, the following boundary condition applies [75]:

$$p_b(0; \sigma, \epsilon, v) dx = p_u(\sigma, \epsilon, v) k_{\text{on}}(\sigma, \epsilon) dt, \quad (2)$$

where $p_u(\sigma, \epsilon, v)$ is the probability of being in the unbound state, and $k_{\text{on}}(\sigma, \epsilon)$ is the bond formation rate. Since bonds in the unbound state are not expected to be affected by the external force or extension, k_{on} is taken to be independent of x . The bound and unbound probabilities satisfy the normalization condition

$$p_u(\sigma, \epsilon, v) + \int_0^\infty p_b(x; \sigma, \epsilon, v) dx = 1. \quad (3)$$

Our NEB calculations (Supplemental Material [26] Sec. V) reveal that the TEBs for both bond rupture and formation, which govern the rates k_{on} and k_{off} , vary linearly with ϵ and σ . In addition, the rupture TEB decreases linearly with the applied lateral force $f = kx$, following the relation $-kxx^*$, where k is the interlayer bond stiffness, and x^* defines a characteristic length scale of the potential barrier [70]. Accordingly, the rates can be expressed using the following Arrhenius-type expressions [23,41,72]:

$$k_{\text{on}}(\sigma, \epsilon) = f_0 \exp \left[- \left(\frac{E_b + \beta_b \sigma + \gamma_b \epsilon}{k_B T} \right) \right],$$

$$k_{\text{off}}(x; \sigma, \epsilon) = g_0 \exp \left[- \left(\frac{E_u + \beta_u \sigma + \gamma_u \epsilon - kxx^*}{k_B T} \right) \right], \quad (4)$$

where f_0 and g_0 are attempt frequencies, E_b and E_u represent the barrier heights for bond formation and rupture, respectively, at zero normal load and EF, $\beta_{b,u}$ are the activation volumes [41] describing the load sensitivity of the activation barrier, $\gamma_{b,u}$ quantify the EF sensitivity of the activation barrier, k_B is the Boltzmann constant, and T is the temperature.

By solving Eqs. (1)–(4) for $p_u(\sigma, \epsilon, v)$ and $p_b(x; \sigma, \epsilon, v)$, we obtain (see Supplemental Material [26] Sec. VI for detailed derivation)

$$p_u(\sigma, \epsilon, v) = \frac{\alpha v}{\alpha v + k_{\text{on}}(\sigma, \epsilon) e^{A(\sigma, \epsilon, v)} \Gamma(0, A(\sigma, \epsilon, v))},$$

$$p_b(x; \sigma, \epsilon, v) = \frac{p_u(\sigma, \epsilon, v) k_{\text{on}}(\sigma, \epsilon)}{v} \exp[-A(\sigma, \epsilon, v)(e^{\alpha x} - 1)], \quad (5)$$

where $\Gamma(0, A) = \int_A^\infty t^{-1} e^{-t} dt$ is the upper incomplete Gamma function [76] $A(\sigma, \epsilon, v) \equiv [(g_0 k_B T)/(x^* v k)] \exp\{[(E_u + \beta_u \sigma + \gamma_u \epsilon)/(k_B T)]\}$, and $\alpha \equiv [(kx^*)/(k_B T)]$. The bond formation probability over the entire sliding trajectory is then straightforwardly estimated as $1 - p_u(\sigma, \epsilon, v)$.

Since chemifrication is governed by the interlayer bonding dynamics, the bonding probability functions derived above can be used to estimate the EF-dependent kinetic lateral stress across varying normal loads and sliding velocities. Using Eq. (5), the average kinetic lateral stress can be calculated as

$$\langle \tau \rangle = \frac{1}{S} \int_0^\infty f(x) p_b(x; \sigma, \epsilon, v) dx, \quad (6)$$

where $f(x) = kx$ is the bond extension force and S is the lateral contact area. The total kinetic lateral stress is the sum of 1B and 2B contributions, though the former dominates (see Fig. 3 and Supplemental Material [26] Videos 1-6).

In twisted incommensurate layered interfaces, the total frictional stress is dominated by chemifrication. Therefore, the stochastic model focuses on ensemble averaged quantities related to independent bond-stretching and rupture events. Equation (6) thus links between the microscopic energy dissipation of individual covalent bonds and the macroscopic frictional response of the entire twisted interface.

Figures 4(a) and 4(b) compare the model predictions [using Eq. (5)] with MD simulation results for the probabilities of one- (“1B”) and two-bond (“2B”) states in the twisted V_0V_3 bilayer as functions of the normal load under EFs ranging from -2 to 2 V/nm at $v = 10$ m/s. In the

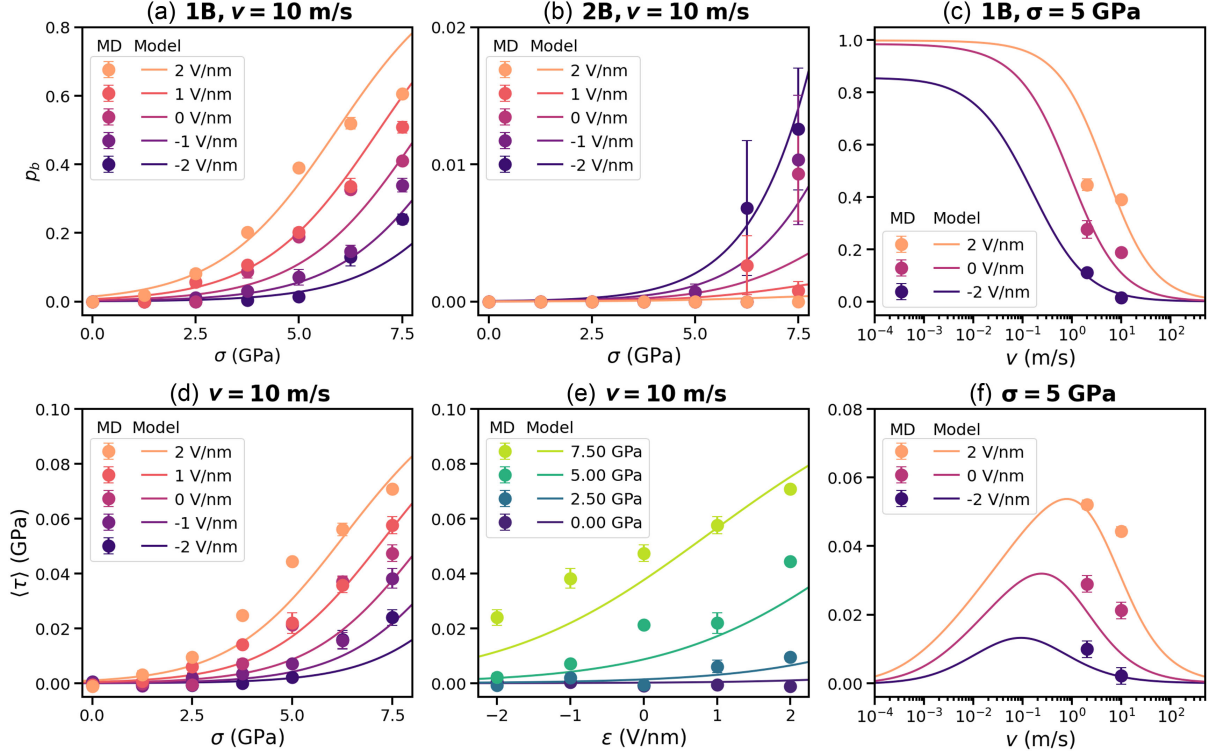


FIG. 4. EF-tunable interlayer bonding probabilities P_b (top panels) and kinetic frictional stress τ (bottom panels) for the twisted V_0V_3 h -BN bilayer at $T = 300$ K. Symbols denote MD simulation results, and solid lines represent the two-state model predictions [panels (a)–(c) using Eq. (5), panels (d)–(f) using Eq. (6)]. The simulation results in panels (a), (b), (d), and (e) are obtained at $v = 10$ m/s. The velocity dependence of friction presented in panels (c) and (f) is obtained at a fixed normal load of $\sigma = 5$ GPa. Panels (a) and (b) show probabilities of the 1B and 2B states as functions of the normal load, respectively. Panel (c) shows the velocity dependence of 1B probability. Panels (d), (e), and (f) show the dependences of kinetic lateral stress on the normal load σ , EF ϵ , and sliding velocity v , respectively. Error bars in all panels represent the standard error of the mean from three independent MD trajectories. Parameter values used in the stochastic model are $f_0 = g_0 = 1000$ ns $^{-1}$, $T = 300$ K, $k = 8$ N/m, $x^* = 0.026$ nm. For the $0P \rightarrow 1B$ transition $E_b = 210$ meV, $\beta_b = -17$ meV/GPa, $\gamma_b = -17$ meV/(V/nm), $E_u = 178$ meV, $\beta_u = 11$ meV/GPa, $\gamma_u = 14$ meV/(V/nm); for the $1B \rightarrow 2B$ transition $E_b = 190$ meV, $\beta_b = -3$ meV/GPa, $\gamma_b = 31$ meV/(V/nm), $E_u = 90$ meV, $\beta_u = 0$ meV/GPa, and $\gamma_u = -11$ meV/(V/nm).

model, the 2B probability is evaluated as the product of the 1B probability and the conditional probability of the $1B \rightarrow 2B$ transition, reflecting the sequential nature of bond formation. The model reproduces the MD trends well across all loads and fields. The TEB heights and the linear response constants of the reaction barriers toward normal load and EF obtained by fitting the model predictions to the MACE MD simulation results are in good agreement with our NEB results at the eclipsed configurations (see Supplemental Material [26] Sec. V for details), with minor deviations arising from the mean-field approximation inherent to the model.

Consistent with our MD simulations, the probability of formation of the 1B state obtained from the two-state model exhibits a strong dependence on the EF across all normal loads, whereas the 2B state appears only at higher loads ($\sigma \geq 5$ GPa). The latter behavior arises from the short lifetime (low rupture barrier) of the $N_1 - B_2$ bond [Fig. 2(b)]. As shown in Fig. 4(c), the probability of the

1B state increases with decreasing velocity, and, according to the model, saturates in the micrometer-per-second regime at 1.00 for $\epsilon = 2$ V/nm, 0.98 for $\epsilon = 0$ V/nm, and 0.86 for $\epsilon = -2$ V/nm.

Our results demonstrate that external EFs act similar to the application of a normal load, such that the application of an increasing positive field enhances friction, similar to the application of a positive normal load. Reversing the direction of the field reduces friction—an effect that is hard to achieve via load modulation alone. At high sliding velocities, the kinetic friction decreases with increasing velocity for all fields considered, reflecting the reduced bond formation probability [Fig. 4(c)].

Given the accuracy of the model in describing the dependence of kinetic friction on normal load and EF [Figs. 4(d) and 4(e)], we employ it to extrapolate the molecular dynamics simulation results to the experimentally relevant low-velocity regime [Fig. 4(f)]. Our results reveal two regimes: At high sliding velocities

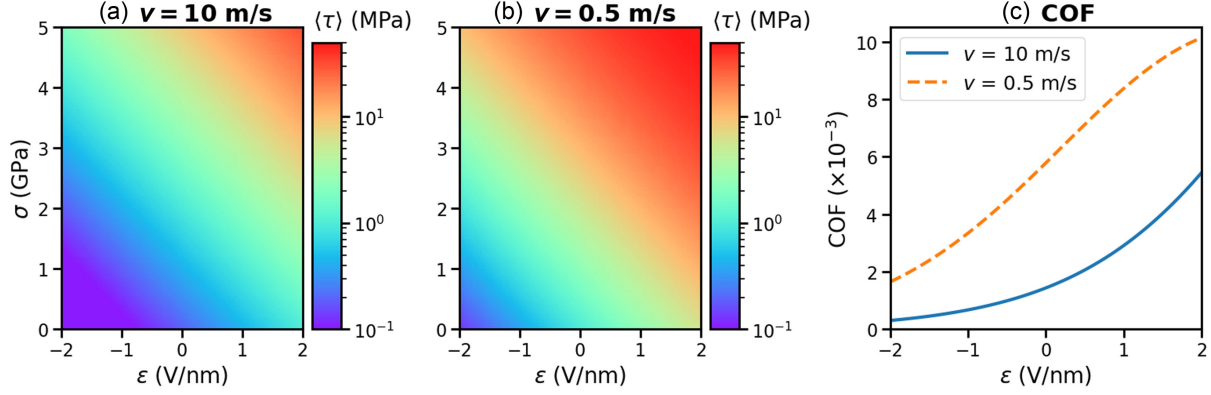


FIG. 5. 2D maps of kinetic frictional stress $\langle \tau \rangle$ for the twisted V_0V_3 h -BN bilayer at $T = 300$ K under sliding velocities of (a) $v = 10$ m/s and (b) $v = 0.5$ m/s. The EF and normal load spans are $\epsilon \in [-2, 2]$ V/nm and $\sigma \in [0, 5]$ GPa, respectively. (c) Corresponding COFs as a function of ϵ calculated for the two velocities. All results were obtained using the stochastic model.

($v > 0.1$ m/s), the chemifrictional stress decreases with increasing velocity because the contact time between reactive sites is too short to allow for significant bond formation. At low sliding velocities, the bond lifetime (approximately 1 μ s) becomes shorter than the characteristic time required for significant bond stretching under shear. Therefore, natural binding and unbinding processes dominate over the effects of chemifriction, such that the chemifrictional stress approaches zero for $v \lesssim 1$ μ m/s. At intermediate velocities (0.1 m/s $\lesssim v \lesssim 1$ m/s), the interfacial bond formation probability is high and stretching is allowed, resulting in increased chemifriction with pronounced EF effect. Compared with the zero-field frictional stress of 0.032 GPa, a positive field of +2 V/nm increases the maximum friction to 0.054 GPa (approximately equal to a 68% increase), whereas a negative field of -2 V/nm reduces it to 0.013 GPa (approximately equal to a 59% decrease). The threshold velocity, below which chemifriction vanishes, decreases with increasing bond lifetime that in turn grows exponentially with the rupture TEB height. For the defected h -BN interfaces studied here, the relatively low rupture barriers (approximately 0.1 eV) yield a threshold velocity of approximately 1 μ m/s. In contrast, it was predicted that in defected twisted-graphene bilayers, where strong interlayer C–C bonds (rupture barriers > 2 eV) dominate frictional response, substantial chemifriction should be observed even at velocities as low as 1 nm/s [23].

Figure 5 presents kinetic frictional stress maps as functions of EF ($\epsilon \in [-2, 2]$ V/nm) and normal load ($\sigma \in [0, 5]$ GPa) for two representative sliding velocities: (i) a high velocity of $v = 10$ m/s used in simulations [Fig. 5(a)] and a lower velocity of $v = 0.5$ m/s [Fig. 5(b)] corresponding to the high-chemifriction regime. Both maps reveal a pronounced reduction of frictional stress when transitioning from positive to negative EF and/or decreasing normal load. Figure 5(c) shows the differential coefficient of friction (COF) calculated from these maps over

the range 0–5 GPa. For $v = 10$ m/s, the COF increases with ϵ from 3.1×10^{-4} at -2 V/nm to 5.5×10^{-3} at $+2$ V/nm. For $v = 0.5$ m/s, the COF rises from 1.6×10^{-3} to 1.0×10^{-2} over the same EF range. These results clearly demonstrate that external EFs enable active and reversible control of chemifriction in defected incommensurate h -BN interfaces, allowing access to the superlubric regime ($\text{COF} \lesssim 10^{-3}$ – 10^{-4} [77]) by appropriately tuning the field strength and direction.

It should be noted that in the aligned V_0V_3 bilayer, EF also strongly modulates interlayer bonding probabilities, exhibiting a qualitatively similar dependence on normal load and sliding velocity (see Supplemental Material [26] Sec. VII). However, in this commensurate configuration, the kinetic friction is dominated by physifriction associated with stick-slip dissipative dynamics arising from interlayer interactions between the pristine h -BN surfaces. Consequently, the overall friction shows only a weak dependence on the applied EF.

VI. CONCLUSIONS

We propose a unique mechanism to control chemifriction (friction induced by interfacial binding) in polar defected layered interfaces using external EFs. Unlike mechanical load, which usually increases bonding and friction by pushing layers together, an external electric field allows for both increasing and decreasing interlayer binding and chemifriction even below the field-free baseline. While mechanical loading affects the entire interface and can cause unwanted wear in pristine areas, EFs are noninvasive and specifically target the reactive bonding sites. Furthermore, the high speed of electrical switching allows for real-time friction control that matches the fast timescales of bond formation and rupture. This provides a level of control that traditional mechanical methods often fail to achieve. The predicted friction tunability is most significant for incommensurate defected interfaces that are

otherwise superlubric. By combining *ab initio* trained MLPs and a stochastic two-state model, we are able to extrapolate our simulation results to the low-velocity regime, thus providing valuable insights for future experimental efforts. The general nature of the EF-tunable bonding mechanism uncovered herein establishes a route to electrically control friction and to reduce wear by suppressing interfacial bond formation. This can be achieved by rational design of asymmetric implantation of structural defects in otherwise pristine interfaces. The proposed framework can be further extended to explore other surface defect configurations and the chemifrictional effects of dangling bonds at surface edges of various layered material interfaces, which, in turn, may affect additional material properties, such as electronic and thermal transport and structural stability.

ACKNOWLEDGMENTS

O. H. would like to thank Dr. Emila Freibrun and the late Prof. Israel Hod for their help and support along the way. O. H. is grateful for the generous financial support of the Heinemann Chair in Physical Chemistry. M. U. is grateful for generous financial support via Grant No. BSF-NSF 2023614.

DATA AVAILABILITY

The MLP data are made available at Zenodo [78], and additional data are available from the corresponding author upon request.

- [1] A. K. Geim and I. V. Grigorieva, *Van der Waals heterostructures*, *Nature (London)* **499**, 419 (2013).
- [2] K. S. Novoselov, A. Mishchenko, A. Carvalho, and A. H. Castro Neto, *2D materials and van der Waals heterostructures*, *Science* **353**, aac9439 (2016).
- [3] Fengnian Xia, Han Wang, Di Xiao, Madan Dubey, and Ashwin Ramasubramaniam, *Two-dimensional material nanophotonics*, *Nat. Photonics* **8**, 899 (2014).
- [4] D. Mandelli, W. Ouyang, M. Urbakh, and O. Hod, *The princess and the nanoscale pea: Long-range penetration of surface distortions into layered materials stacks*, *ACS Nano* **13**, 7603 (2019).
- [5] W. Ouyang, O. Hod, and M. Urbakh, *Parity-dependent moire superlattices in graphene/h-BN heterostructures: A route to mechanomutable metamaterials*, *Phys. Rev. Lett.* **126**, 216101 (2021).
- [6] M. Dienwiebel, G. S. Verhoeven, N. Pradeep, Joost W. Frenken, J. A. Heimberg, and H. W. Zandbergen, *Superlubricity of graphite*, *Phys. Rev. Lett.* **92**, 126101 (2004).
- [7] A. E. Filippov, M. Dienwiebel, Joost W. Frenken, J. Klafter, and M. Urbakh, *Torque and twist against superlubricity*, *Phys. Rev. Lett.* **100**, 046102 (2008).
- [8] D. Mandelli, W. Ouyang, O. Hod, and M. Urbakh, *Negative friction coefficients in superlubric graphite-hexagonal boron nitride heterojunctions*, *Phys. Rev. Lett.* **122**, 076102 (2019).
- [9] Jin Wang, Ali Khosravi, Andrea Vanossi, and Erio Tosatti, *Colloquium: Sliding, and pinning in structurally lubric 2D material interfaces*, *Rev. Mod. Phys.* **96**, 011002 (2024).
- [10] L. J. Li, E. C. O'Farrell, K. P. Loh, G. Eda, B. Ozyilmaz, and A. H. Castro Neto, *Controlling many-body states by the electric-field effect in a two-dimensional material*, *Nature (London)* **529**, 185 (2016).
- [11] S. K. Srivastav, A. Udupa, K. Watanabe, T. Taniguchi, D. Sen, and A. Das, *Electric-field-tunable edge transport in bernal-stacked trilayer graphene*, *Phys. Rev. Lett.* **132**, 096301 (2024).
- [12] Y. Wang, J. Wang, T. Wu, W. Chen, D. Peng, Z. Wu, M. Ma, and Q. Zheng, *The anomalous effect of electric field on friction for microscale structural superlubric graphite/Au contact*, *Natl. Sci. Rev.* **11**, nwae019 (2024).
- [13] Diana Berman, Leonardo Israel Farfan-Cabrera, Andreas Rosenkranz, and Ali Erdemir, *2D materials for durable, and sustainable electric vehicles*, *Nat. Rev. Mater.* **9**, 527 (2024).
- [14] S. Shaik, R. Ramanan, D. Danovich, and D. Mandal, *Structure and reactivity/selectivity control by oriented-external electric fields*, *Chem. Soc. Rev.* **47**, 5125 (2018).
- [15] M. Vizner Stern, Y. Waschitz, W. Cao, I. Nevo, K. Watanabe, T. Taniguchi, E. Sela, M. Urbakh, O. Hod, and M. Ben Shalom, *Interfacial ferroelectricity by van der Waals sliding*, *Science* **372**, 1462 (2021).
- [16] S. Deb, W. Cao, N. Raab, K. Watanabe, T. Taniguchi, M. Goldstein, L. Kronik, M. Urbakh, O. Hod, and M. Ben Shalom, *Cumulative polarization in conductive interfacial ferroelectrics*, *Nature (London)* **612**, 465 (2022).
- [17] Zhaokuan Yu, Jinbo Bian, Jin Wang, Zonghuiyi Jiang, Xuanyu Huang, Linxin Zhai, Xin Lu, Xiaofei Liu, Quanshui Zheng, and Zhiping Xu, *On-device control of electronic friction*, *Phys. Rev. X* **16**, 011050 (2026).
- [18] Florian Banhart, Jani Kotakoski, and Arkady V. Krasheninnikov, *Structural defects in graphene*, *ACS Nano* **5**, 26 (2011).
- [19] X. Gao, M. Urbakh, and O. Hod, *Stick-slip dynamics of moire superstructures in polycrystalline 2D material interfaces*, *Phys. Rev. Lett.* **129**, 276101 (2022).
- [20] J. H. Jeong, Y. Jung, J. U. Park, and G. H. Lee, *Gate-tunable electrostatic friction of grain boundary in chemical-vapor-deposited MoS(2)*, *Nano Lett.* **23**, 3085 (2023).
- [21] Penghua Ying, Xiang Gao, Diana Berman, Oded Hod, and Michael Urbakh, *Scaling-up of structural superlubricity: Challenges, and opportunities*, *Adv. Funct. Mater.* **35**, 2423024 (2025).
- [22] Penghua Ying, Amir Natan, Oded Hod, and Michael Urbakh, *Effect of interlayer bonding on superlubric sliding of graphene contacts: A machine-learning potential study*, *ACS Nano* **18**, 10133 (2024).
- [23] Penghua Ying, Xiang Gao, Amir Natan, Michael Urbakh, and Oded Hod, *Chemifriction, and superlubricity: Friends or foes?*, *J. Phys. Chem. Lett.* **16**, 2934 (2025).
- [24] G. H. Ryu, H. J. Park, J. Ryoo, J. Park, J. Lee, G. Kim, H. S. Shin, C. W. Bielawski, R. S. Ruoff, S. Hong, and Z. Lee, *Atomic-scale dynamics of triangular hole growth in monolayer hexagonal boron nitride under electron irradiation*, *Nanoscale* **7**, 10600 (2015).
- [25] H. Park, Y. Wen, S. X. Li, W. Choi, G. D. Lee, M. Strano, and J. H. Warner, *Atomically precise control of carbon*

- insertion into hBN monolayer point vacancies using a focused electron beam guide, *Small* **17**, e2100693 (2021).
- [26] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/s32x-hjrx> for additional information on the energy barrier for interlayer binding dynamics in various defected bilayers, DFT calculations, MLP training and validation, reactive sliding dynamics production simulation setup, bond formation and rupture barriers under EFs and normal loads, detailed derivation of Eq. (5), and physifriction and chemifriction of h-BN bilayers from sliding dynamics simulations. Supplemental Material includes Refs. [22,27–47].
- [27] Graeme Henkelman, Blas P Uberuaga, and Hannes Jónsson, *A climbing image nudged elastic band method for finding saddle points, and minimum energy paths*, *J. Chem. Phys.* **113**, 9901 (2000).
- [28] Georg Kresse and Jürgen Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, *Phys. Rev. B* **54**, 11169 (1996).
- [29] Georg Kresse and Daniel Joubert, *From ultrasoft pseudopotentials to the projector augmented-wave method*, *Phys. Rev. B* **59**, 1758 (1999).
- [30] Ask Hjorth Larsen, Jens Jørgen Mortensen, Jakob Blomqvist, Ivano E Castelli, Rune Christensen, Marcin Dułak, Jesper Friis, Michael N Groves, Bjørk Hammer, and Cory Hargus, *The atomic simulation environment—a Python library for working with atoms*, *J. Phys. Condens. Matter* **29**, 273002 (2017).
- [31] P. E Blöchl, *Projector augmented-wave method*, *Phys. Rev. B* **50**, 17953 (1994).
- [32] Stefan Grimme, Stephan Ehrlich, and Lars Goerigk, *Effect of the damping function in dispersion corrected density functional theory*, *J. Comput. Chem.* **32**, 1456 (2011).
- [33] Ilyes Batatia, David P Kovacs, Gregor Simm, Christoph Ortner, and Gábor Csányi, *MACE: Higher order equivariant message passing neural networks for fast, and accurate force fields*, in *Advances in Neural Information Processing Systems* (Curran Associates, Inc., Red Hook, NY, 2022), p. 11423.
- [34] Penghua Ying, Cheng Qian, Rui Zhao, Yanzhou Wang, Ke Xu, Feng Ding, Shunda Chen, and Zheyong Fan, *Advances in modeling complex materials: The rise of neuroevolution potentials*, *Chem. Phys. Rev.* **6**, 011310 (2025).
- [35] D. P. Kovacs, I. Batatia, E. S. Arany, and G. Csanyi, *Evaluation of the MACE force field architecture: From medicinal chemistry to materials science*, *J. Chem. Phys.* **159**, 044118 (2023).
- [36] Diederik P Kingma and Jimmy Ba, *Adam: A method for stochastic optimization*, [arXiv:1412.6980](https://arxiv.org/abs/1412.6980).
- [37] Afshin Zamani zakaria, *A two-section beam element to model the B-N covalent bonds in boron nitride nanotubes*, *Mater. Res. Bull.* **145**, 111533 (2022).
- [38] T Schneider and E Stoll, *Molecular-dynamics study of a three-dimensional one-component model for distortive phase transitions*, *Phys. Rev. B* **17**, 1302 (1978).
- [39] <https://github.com/ACEsuit/mace> (Accessed 2025-09-03).
- [40] Tevis D. B. Jacobs, Bernd Gotsmann, Mark A. Lantz, and Robert W. Carpick, *On the application of transition state theory to atomic-scale wear*, *Tribol. Lett.* **39**, 257 (2010).
- [41] Ashlie Martini and Seong H. Kim, *Activation volume in shear-driven chemical reactions*, *Tribol. Lett.* **69**, 150 (2021).
- [42] Ashlie Martini and Seong H. Kim, *Correction to: Activation volume in shear-driven chemical reactions*, *Tribol. Lett.* **71**, 14 (2022).
- [43] B. Gotsmann and M. A. Lantz, *Atomistic wear in a single asperity sliding contact*, *Phys. Rev. Lett.* **101**, 125501 (2008).
- [44] S. Kadhodaei and A. van de Walle, *A simple local expression for the prefactor in transition state theory*, *J. Chem. Phys.* **150**, 144105 (2019).
- [45] J. Lefèvre López, N. Mousseau, G. Adjanor, and C. Domain, *Harmonic transition state theory applied to vacancy diffusion pre-exponential factors in a concentrated solid-solution alloy*, *Phys. Rev. Mater.* **8**, 013609 (2024).
- [46] Abraham Savitzky and M. J. E. Golay, *Smoothing and differentiation of data by simplified least squares procedures*, *Anal. Chem.* **36**, 1627 (1964).
- [47] P. Virtanen *et al.* (SCIPY Contributors), *SCIPY 1.0: Fundamental algorithms for scientific computing in Python*, *Nat. Methods* **17**, 261 (2020).
- [48] John P Perdew, Kieron Burke, and Matthias Ernzerhof, *Generalized gradient approximation made simple*, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [49] Alexander Stukowski, *Visualization, and analysis of atomistic simulation data with OVITO—the open visualization tool*, *Model. Simul. Mater. Sci. Eng.* **18**, 015012 (2010).
- [50] O. Hod, *Graphite and hexagonal boron-nitride have the same interlayer distance. Why?*, *J. Chem. Theory Comput.* **8**, 1360 (2012).
- [51] Fabian Ducry, Dominic Waldhoer, Theresia Knobloch, Miklos Csontos, Nadia Jimenez Olalla, Juerg Leuthold, Tibor Grasser, and Mathieu Luisier, *An ab initio study on resistance switching in hexagonal boron nitride*, *npj 2D Mater. Appl.* **6**, 58 (2022).
- [52] Manuel Guidon, Jürg Hutter, and Joost VandeVondele, *Robust periodic Hartree–Fock exchange for large-scale simulations using Gaussian basis sets*, *J. Chem. Theory Comput.* **5**, 3010 (2009).
- [53] J. Behler and M. Parrinello, *Generalized neural-network representation of high-dimensional potential-energy surfaces*, *Phys. Rev. Lett.* **98**, 146401 (2007).
- [54] V. L. Deringer, M. A. Caro, and G. Csanyi, *Machine learning interatomic potentials as emerging tools for materials science*, *Adv. Mater.* **31**, 1902765 (2019).
- [55] O. T. Unke, S. Chmiela, H. E. Sauceda, M. Gastegger, I. Poltavsky, K. T. Schütt, A. Tkatchenko, and K. R. Müller, *Machine learning force fields*, *Chem. Rev.* **121**, 10142 (2021).
- [56] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, *J. Comput. Phys.* **285**, 316 (2015).
- [57] Alexander V. Shapeev, *Moment tensor potentials: A class of systematically improvable interatomic potentials*, *Multi-scale Model. Simul.* **14**, 1153 (2016).
- [58] Stefan Chmiela, Alexandre Tkatchenko, Huziel E. Sauceda, Igor Poltavsky, Kristof T. Schütt, and Klaus-Robert Müller,

- Machine learning of accurate energy-conserving molecular force fields*, *Sci. Adv.* **3**, e1603015 (2017).
- [59] A. P. Bartok, M. C. Payne, R. Kondor, and G. Csanyi, *Gaussian approximation potentials: The accuracy of quantum mechanics, without the electrons*, *Phys. Rev. Lett.* **104**, 136403 (2010).
- [60] Zheyong Fan, Zezhu Zeng, Cunzhi Zhang, Yanzhou Wang, Keke Song, Haikuan Dong, Yue Chen, and Tapio Ala-Nissila, *Neuroevolution machine learning potentials: Combining high accuracy, and low cost in atomistic simulations, and application to heat transport*, *Phys. Rev. B* **104**, 104309 (2021).
- [61] L. Zhang, J. Han, H. Wang, R. Car, and E. W. *Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics*, *Phys. Rev. Lett.* **120**, 143001 (2018).
- [62] Z. Fan *et al.*, *GPUMD: A package for constructing accurate machine-learned potentials, and performing highly efficient atomistic simulations*, *J. Chem. Phys.* **157**, 114801 (2022).
- [63] S. Batzner, A. Musaelian, L. Sun, M. Geiger, J. P. Mailoa, M. Kornbluth, N. Molinari, T. E. Smidt, and B. Kozinsky, *E (3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials*, *Nat. Commun.* **13**, 2453 (2022).
- [64] J. Behler, *Perspective: Machine learning potentials for atomistic simulations*, *J. Chem. Phys.* **145**, 170901 (2016).
- [65] J. Kikkawa, C. Shinei, J. Chen, Y. Masuyama, Y. Yamazaki, T. Mizoguchi, K. Kimoto, T. Taniguchi, and T. Teraji, *Observation of boron vacancy concentration in hexagonal boron nitride at nanometer scale*, *Nano Lett.* **25**, 13191 (2025).
- [66] Fei Ren, Zongwei Xu, and Yiyuan Wu, *Optimization of carbon irradiation parameters for creating spin defects in hexagonal boron nitride*, *Nanotechnol. Precis. Eng.* **8**, 033014 (2025).
- [67] Aidan P Thompson, H Metin Aktulga, Richard Berger, Dan S Bolintineanu, W Michael Brown, Paul S Crozier, Pieter J in't Veld, Axel Kohlmeyer, Stan G Moore, and Trung Dac Nguyen, *LAMMPS-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales*, *Comput. Phys. Commun.* **271**, 108171 (2022).
- [68] T. Sun, E. Gao, X. Jia, J. Bian, Z. Wang, M. Ma, Q. Zheng, and Z. Xu, *Robust structural superlubricity under gigapascal pressures*, *Nat. Commun.* **15**, 5952 (2024).
- [69] M. Han, D. Peng, D. Yang, J. Wang, Y. Zheng, G. Hu, Y. Shao, J. Li, F. Ding, Z. Xu, M. Urbakh, and Q. Zheng, *Observation of robust macroscale structural superlubricity*, *Phys. Rev. Lett.* **136**, 076201 (2026).
- [70] Hendrik Anthony Kramers, *Brownian motion in a field of force, and the diffusion model of chemical reactions*, *Physica* **7**, 284 (1940).
- [71] C. Tang, Y. Jiang, C. Chen, C. Xiao, J. Sun, L. Qian, and L. Chen, *Graphene failure under MPa: Nanowear of step edges initiated by interfacial mechanochemical reactions*, *Nano Lett.* **24**, 3866 (2024).
- [72] W. Ouyang, S. N. Ramakrishna, A. Rossi, M. Urbakh, N. D. Spencer, and A. Arcifa, *Load and velocity dependence of friction mediated by dynamics of interfacial contacts*, *Phys. Rev. Lett.* **123**, 116102 (2019).
- [73] L. Caputo, V. H. Nguyen, and J. C. Charlier, *First-principles study of the structural and electronic properties of BN-ring doped graphene*, *Phys. Rev. Mater.* **6**, 114001 (2022).
- [74] Yalin Dong, Qunyang Li, and Ashlie Martini, *Molecular dynamics simulation of atomic friction: A review, and guide*, *J. Vac. Sci. Technol. A* **31**, 030801 (2013).
- [75] Pierre Sens, *Rigidity sensing by stochastic sliding friction*, *Europhys. Lett.* **104**, 38003 (2013).
- [76] Larry C Andrews, *Special Functions of Mathematics for Engineers* (Spie Press, Bellingham, WA, 1998), Vol. 49.
- [77] O. Hod, E. Meyer, Q. Zheng, and M. Urbakh, *Structural superlubricity and ultralow friction across the length scales*, *Nature (London)* **563**, 485 (2018).
- [78] P. Ying, *Electric-Field Control of Interlayer Binding and Friction in h-BN Contacts*, Version v1, [dataset], Zenodo, 2026, 10.5281/zenodo.18151591.