

Robust Superlubricity in Graphene/*h*-BN Heterojunctions

Supporting Information

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Strained unit cell calculations

For the definition of the registry index given in the main text we have used a strained graphene/*h*-BN bilayer unit-cell where the lattice vectors of both layers are forced to be identical. The strained unit-cell was constructed at the optimal C stacking mode with an interlayer distance of 3.3 Å in accordance with the results of Sachs *et al.*¹ obtained using the adiabatic connection fluctuation-dissipation theorem within the random phase approximation (ACFDT-RPA). Applying two dimensional periodic boundary conditions the system's geometry was optimized using density functional theory (DFT) calculations at the HSE/6-31G* level of theory.²⁻⁸ Since we do not use a dispersion corrected functional approximation the interlayer distance was fixed at its initial value during the optimization process. The optimized structure is depicted in Fig. S1 where the inter-atomic distance obtained is $L_{CC} = L_{BN} = 1.431$ Å which is approximately the average value between the inter-atomic separations of the individual layers $L_{CC}=1.42$ Å and $L_{BN}=1.446$ Å. The sliding energy surface of the strained graphene/*h*-BN bilayer system presented in Fig. 2(a) of the main text was obtained by performing relative interlayer lateral shifts of the optimized coordinates and conducting single point calculations at each interlayer configuration.

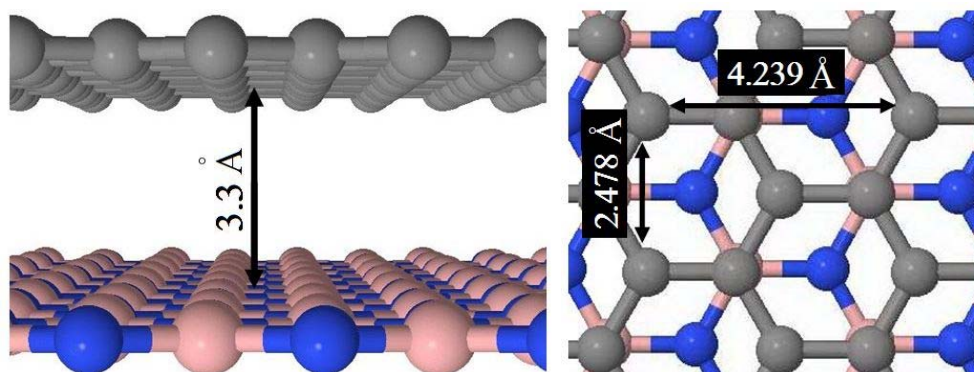


Figure S1: Schematic representation of the optimized strained graphene/*h*-BN system. The interlayer distance was kept fixed at 3.3 Å.

The optimized coordinates of the strained unit-cell with a fixed interlayer distance of 3.3 Å are given below:

| Atom \ Axis | X | Y | Z |
|----------------------|-----------|-----------|-----|
| N | -0.617303 | -0.336971 | 0.0 |
| B | 0.621933 | 0.378571 | 0.0 |
| C | -0.617401 | -1.77737 | 3.3 |
| C | 0.622006 | -1.061760 | 3.3 |
| T_v | 2.478620 | 0.00029 | 0.0 |
| T_v | 1.239341 | 2.146468 | 0.0 |

We note that throughout the paper we neglect possible out of plane corrugation of both graphene and *h*-BN layers as these are expected to be of marginal effect.¹

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