Supporting Information

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First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials

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Computational details are accessible via: http://dx.doi.org/10.17632/yrn7p7w37f.1

Which contains:

*Important Notes.pdf* which contains important information for straightforward training of MTPs and details of various folders.

*LAMMPS-Inputs.zip* folder includes: four examples of LAMMPS input scripts to study the mechanical properties at 300 K with the MTPs interatomic potentials.

*AIMD-Inputs.zip* folder includes: VASP input parameters for the AIMD simulations.

*POSCARs-for-AIMD.zip* folder includes: all considered structures for AIMD calculations.

*Heterostructure-Models.zip* folder includes: constructed four graphene/borophene heterostructure models.

*Training-Data-Full.zip* folder includes: full obtained AIMD trajectories.

*Clean-MTP.zip* folder includes: untrained MTPs.

*FEM-ABAQUS-Models.zip* folder includes: examples of ABAQUS input files for two heterostructures with the domain size of 63 μm (ABAQUS version 6.20).
Fig. S1, Phonon dispersion relations of graphene by DFPT (red-dotted lines) method and trained MTP (continuous green lines) under different biaxial strains ($\varepsilon_{\text{biaxial}}$).
Fig. S2, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.

Fig. S3, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.

Fig. S4, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.
**Fig. S5**, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.

**Fig. S6**, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.

**Fig. S7**, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.
Fig. S8, MTP-based CMD results for the uniaxial stress-strain response and deformation of a heterostructure with the illustrated interface at room temperature. The color coding represents the out-of-plane displacement at each strain level.

Fig. S9, MTP-based CMD results for the uniaxial stress-strain response of pristine graphene and borophene at room temperature at different [strain rates].
Fig. S10. Construction of Voronoi based polycrystalline models of heterostructures in ABAQUS/standard.