molecules

MDPI

Supporting Information

Two-dimensional TeB Structures with Anisotropic Carrier Mobility and Tunable Bandgap

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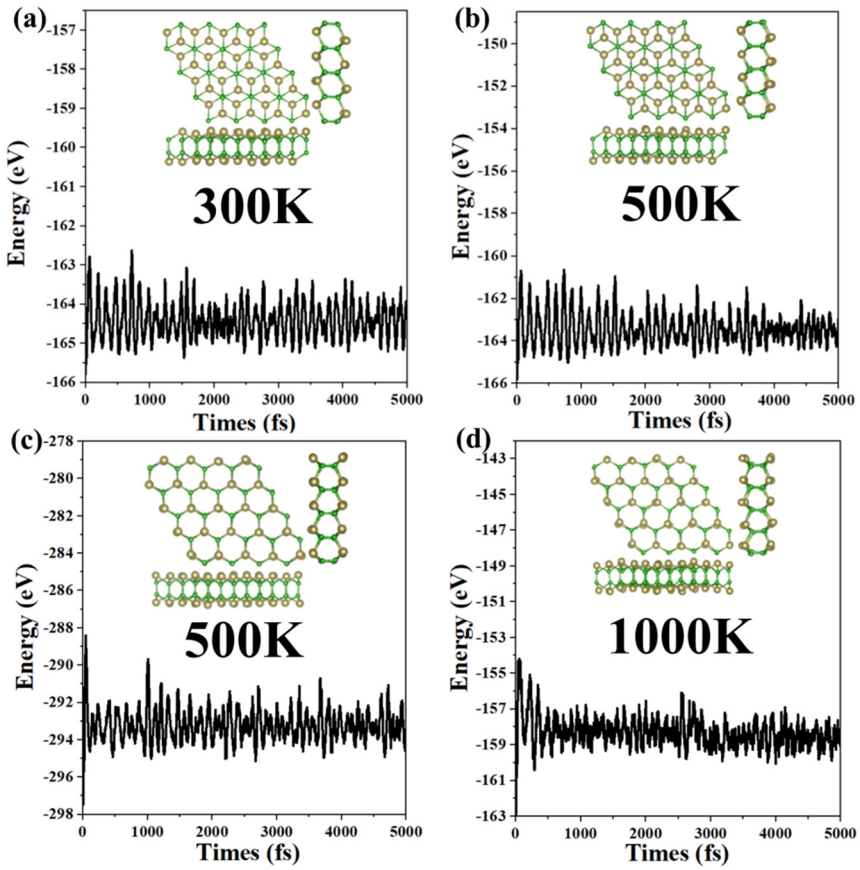

Figure S1. The energy fluctuation and the corresponding structure during the AIMD simulations at 300 K(**a**) and 500 K(**b**) for α-TeB, 500K(**c**) and 1000 K(**d**) for β-TeB, respectively.

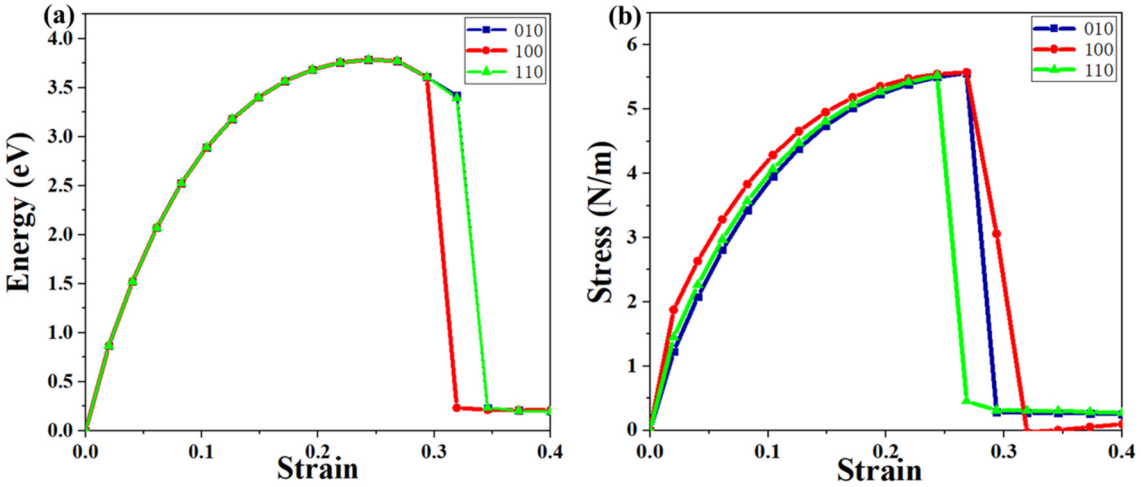

Figure S2. The ideal strength of α-TeB (**a**) and β-TeB (**b**) monolayers, respectively.

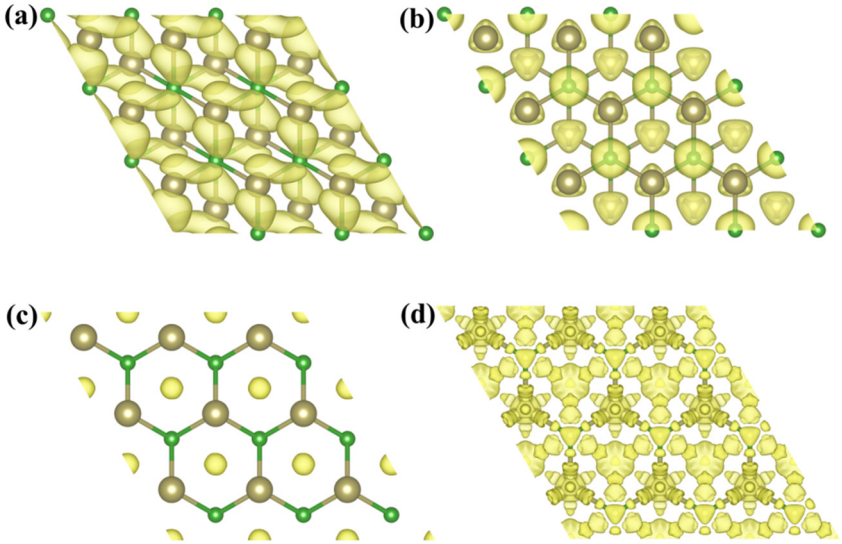

Figure S3. The band decomposed charge densities for VBM (**a**) and CBM (**b**) of α-TeB monlayer and The band decomposed charge densities for VBM (**c**) and CBM (**d**) of β-TeB monlayer.