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Transition from Indirect Type-I to Direct Type-II Bandgaps in α-tellurene/$Ca(OH)_2$ Heterostructure with Superb Optical Properties

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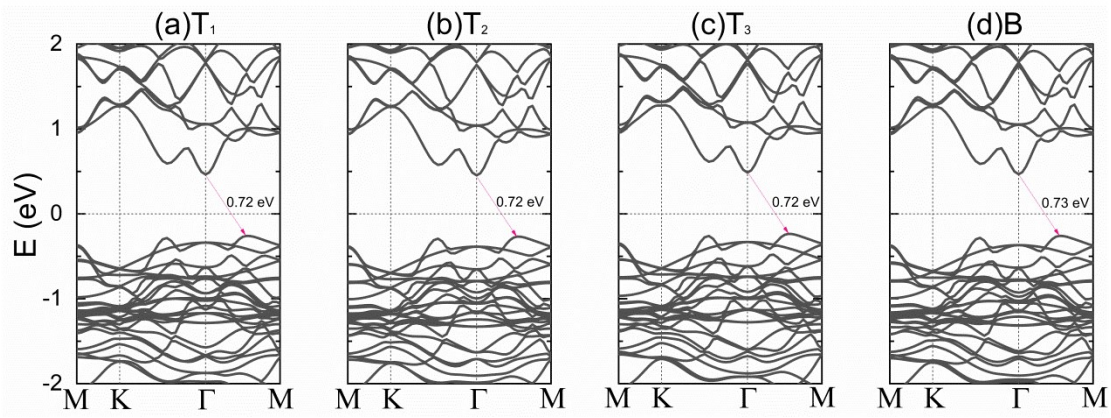
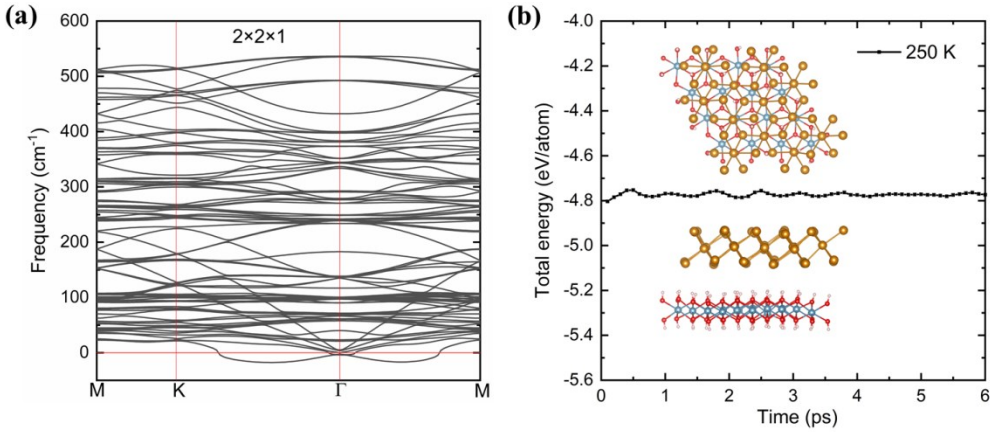
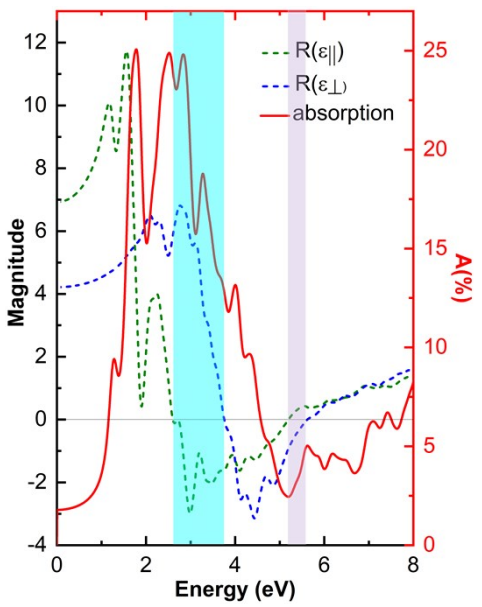


Figure S1. Band structures of the Te/$Ca(OH)_2$ bilayer with four different configurations by PBE functional. Here, the Fermi levels are set to zero.



Figuer S2. (a) Phonon dispersion spectra of the Te/$Ca(OH)_2$ vdWH for a 2×2×1 supercell, respectively. (b) Evolution of the average total energy per atom with time in the AIMD simulation. Thereinto, the insets are the top and side views of final structure obtained from the AIMD simulations.



Figsure S3. (a) Real parts of permittivity and (b) optical absorption of the Te/Ca(OH)2 vdWH obtained from HSE06 functional.

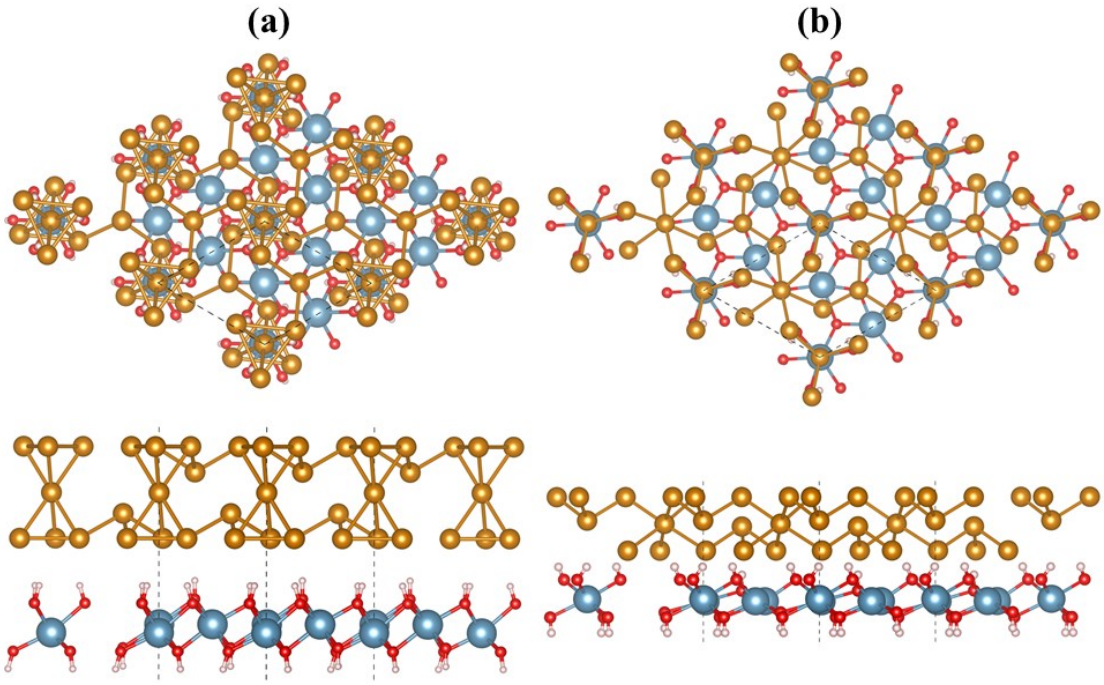


Figure S4. Top and side views of the crystal structures of the Te/$Ca(OH)_2$ heterobilayer under the applied strain of (a) -9% and (b) 14%, respectively.