RESEARCH ARTICLE

Strain-triggered high-temperature superconducting transition in two-dimensional carbon allotrope

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Supporting Information

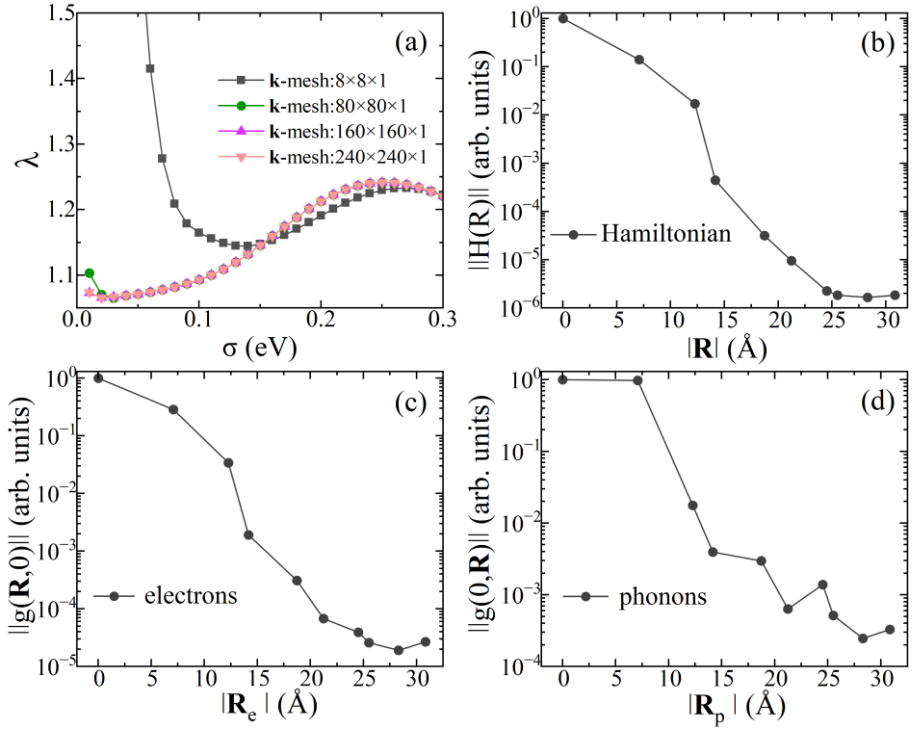

Figure S1. (a) Convergence test of EPC constant versus smearing parameter σ in THO-graphene under 12% strain. Fine phonon grid is chosen to be 80×80×1. (b) Spatial decay of the electronic Hamiltonian in Wannier representation. (c) and (d) Spatial decays of EPC matrix elements in Wannier representation. Data in (b)-(d) are normalized by their respective maximum values.

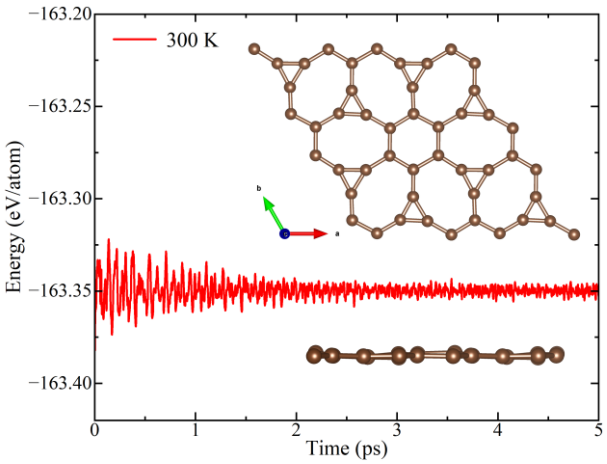

Figure S2. Time evolution of the total energy per atom in the THO-graphene at 300 K obtained in *ab initio* molecular dynamics. The insets show the top and side views of the final snapshot at 5 ps.

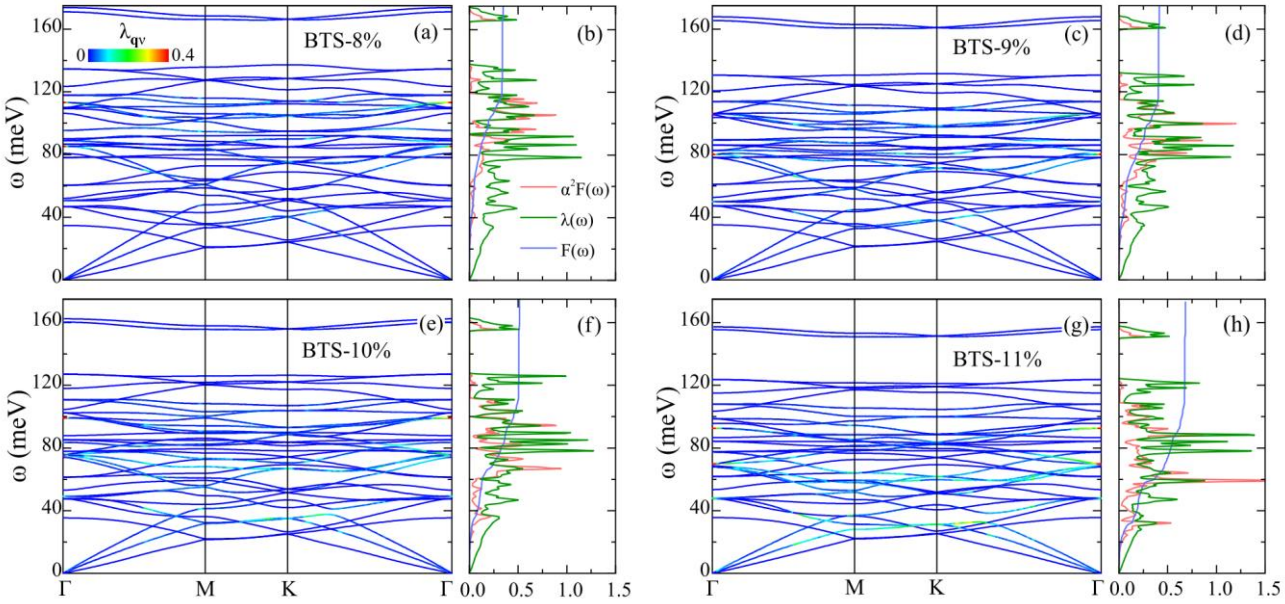

Figure S3. Lattice dynamics of THO-graphene under BTS of 8%, 9%, 10%, and 11%. (a), (c), (e), (g) Phonon spectra at different BTS. Colors represent the strength of EPC constant λ_{qv} for phonon mode **q**v. (b), (d), (f), (h) Phonon density of states F(ω) (modes/meV), Eliashberg spectral functions $\alpha^2F(\omega)$ and λ(ω).

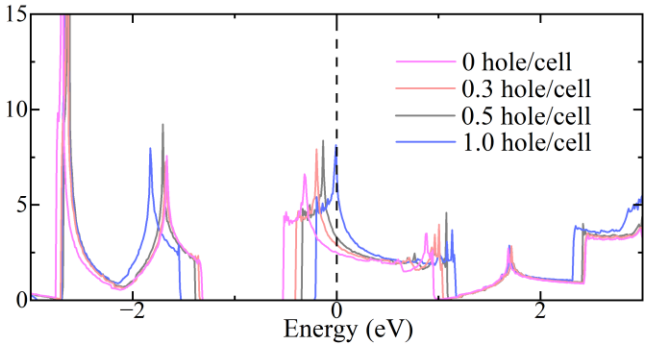

Figure S4. Density of states under different doping concentrations at BTS of 12%.

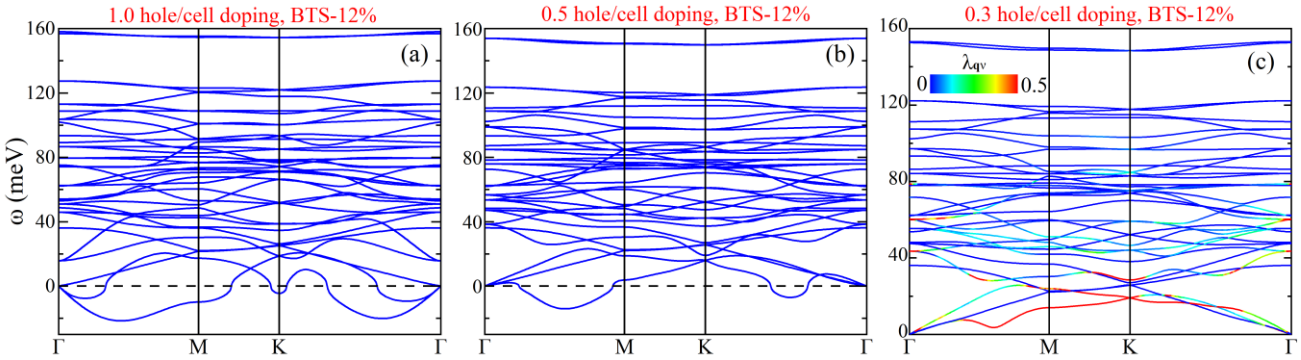

Figure S5. Phonon spectra at different doping concentrations under 12% BTS. The strengths of λ_{qv} are mapped by different colors for 0.3 hole/cell doped THO-graphene.

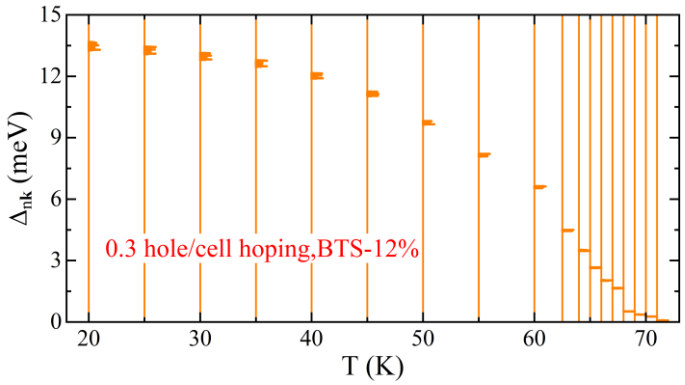

Figure S6. Temperature dependence of the superconducting gap Δ_{nk} under doping concentration of 0.3 hole/cell and 12% BTS.

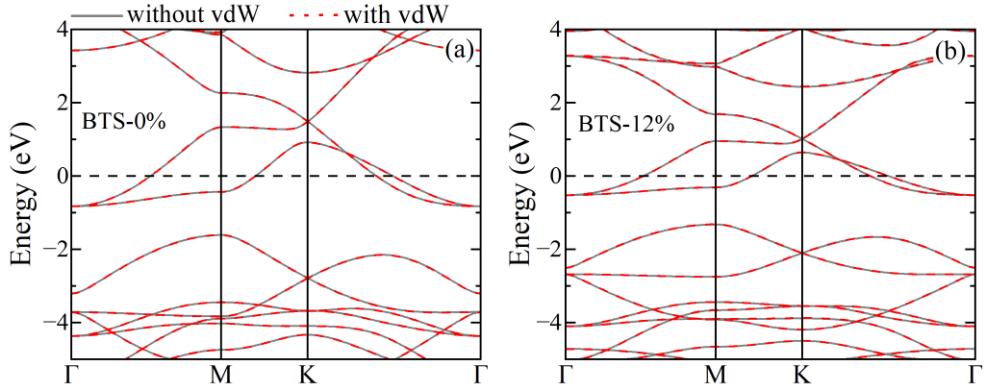

Figure S7. Band structures for the unstrained and 12%-strained THO-graphene with (dashed lines) and without (solid lines) vdW correction.

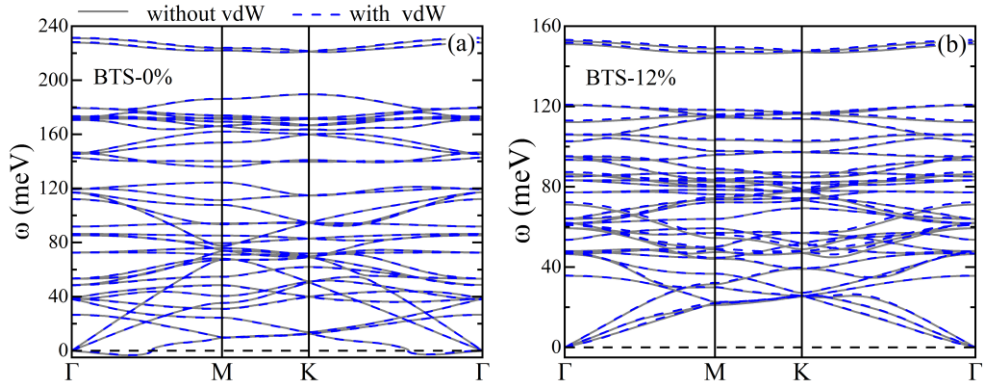

Figure S8. Phonon spectra for the unstrained and 12%-strained THO-graphene with (dashed lines) and without (solid lines) vdW correction.

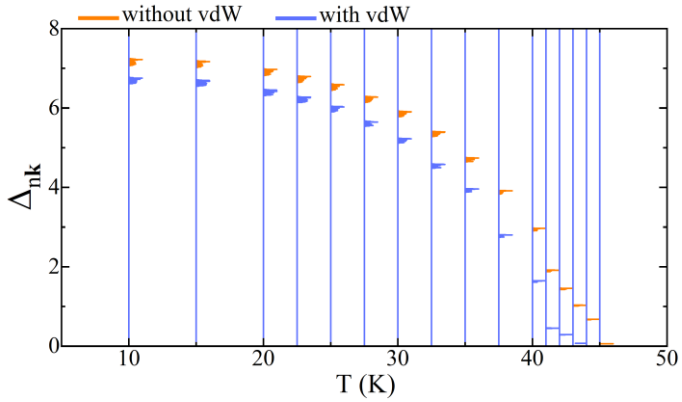

Figure S9. Superconducting gap distribution versus temperature under 12% strain. Orange and blue curves represent the results without and with vdW correction, respectively.

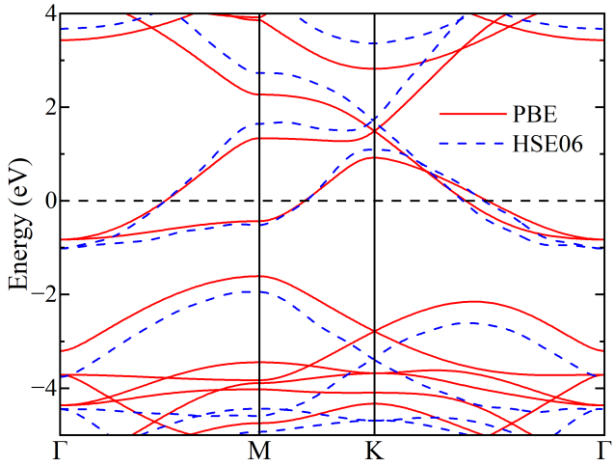

Figure S10. Band structure calculated with HSE06 hybrid functional for free-standing THO-graphene.

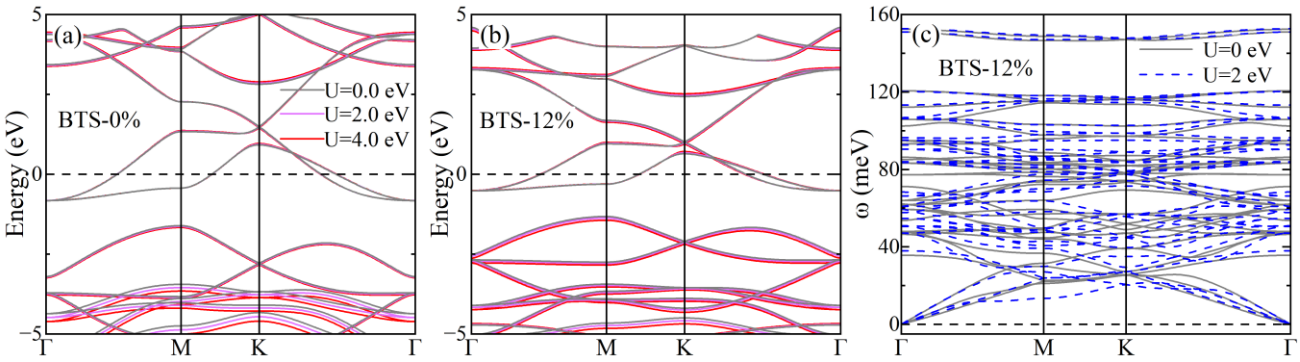

Figure S11. Influences of strong correlation on electronic structures and phonons of THO-graphene. Band structures of free-standing (a) and 12%-strained THO-graphene (b) under different U values. (c) Phonon spectra comparison for 12%-strained THO-graphene with and without the inclusion of U=2.0 eV.