

Supplementary information

Is graphitic silicon carbide (silagraphene) stable?

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Fig. S1. Close-up of the total electron density map for the AA' stacking with a larger supercell which clearly shows the sandwich arrangement

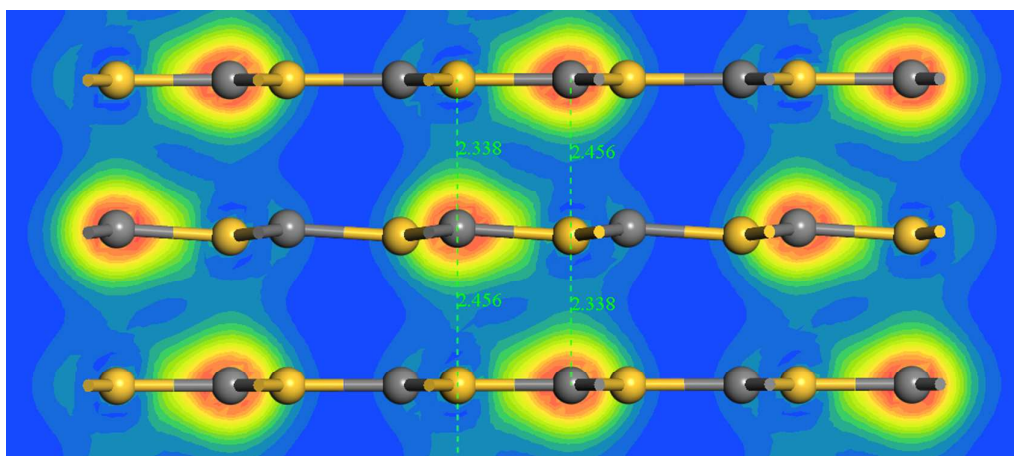


Fig. S2. Energy minimization curve using the density mixing approach for AA' stacking

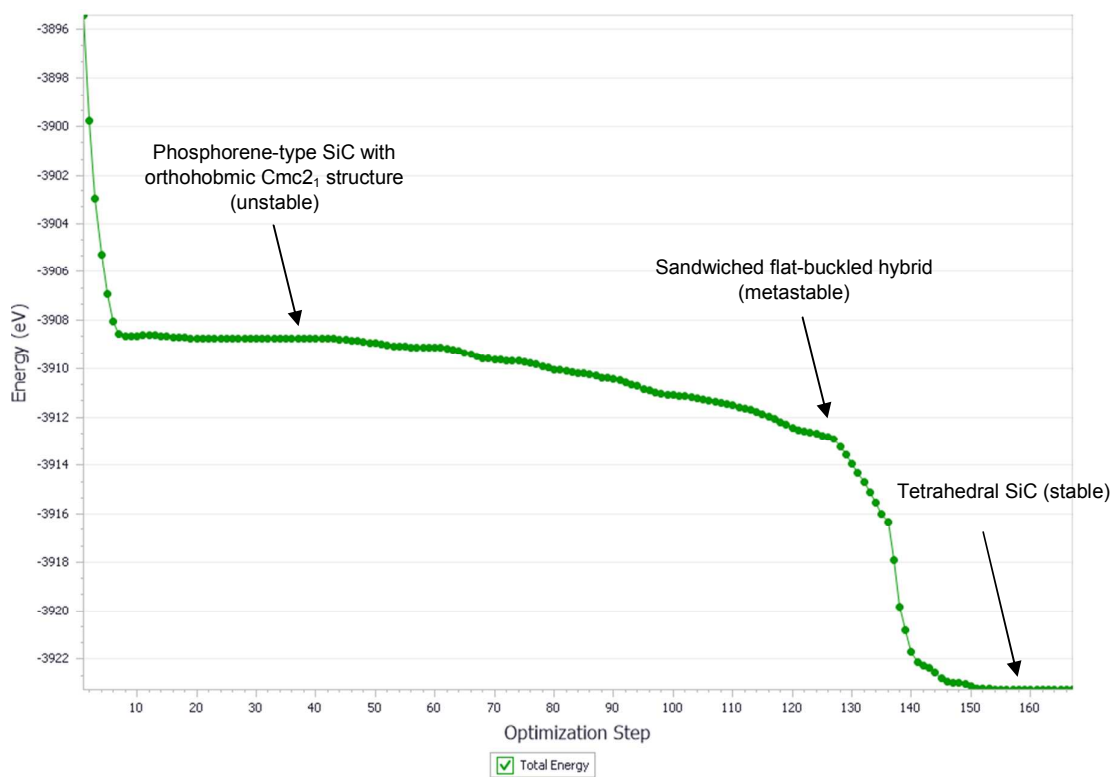


Fig. S3. The phosphorene-type SiC with orthorhombic Cmc2₁ structure (unstable AA')

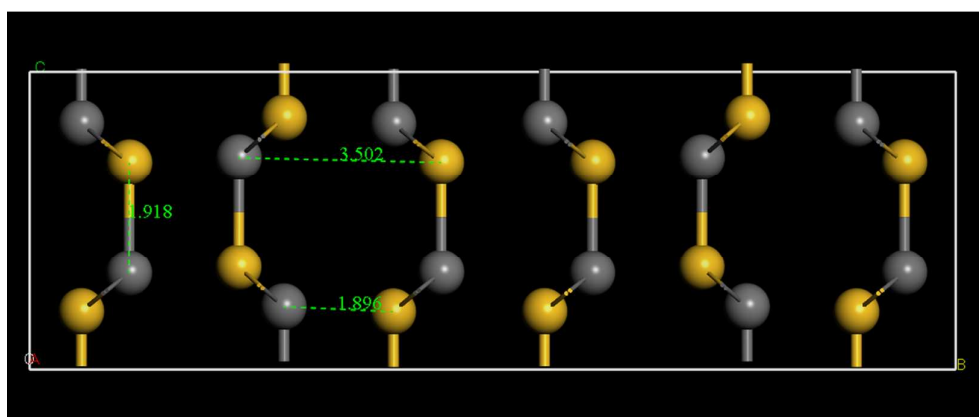


Fig. S4. Imaginary acoustic modes in the phonon dispersion of the sandwiched flat-buckled hybrid (metastable AA')

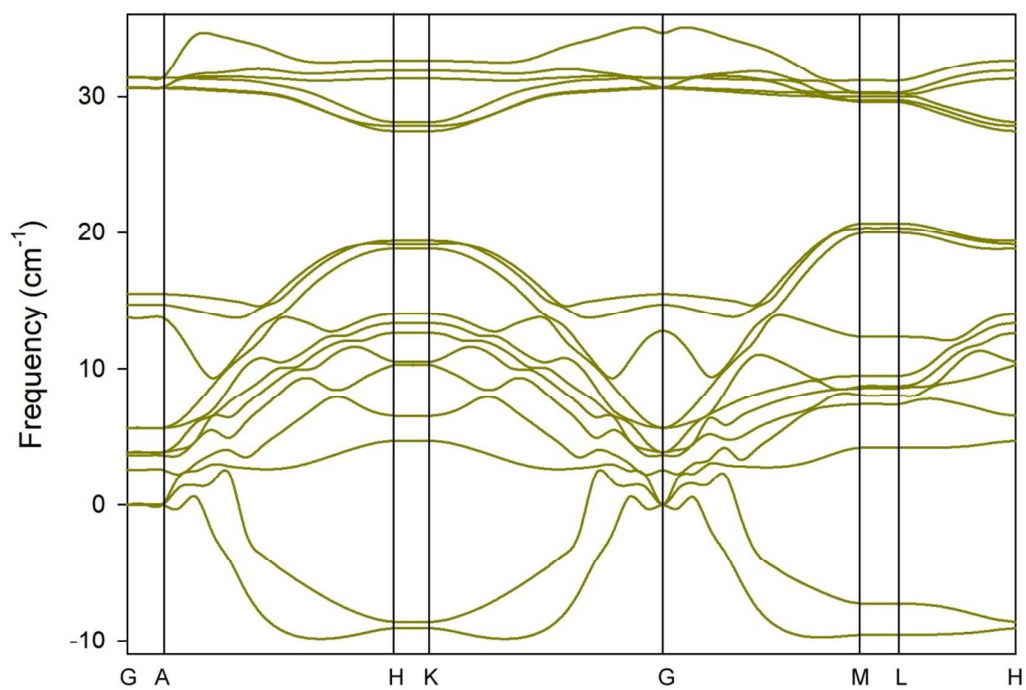


Fig. S5. Phonon dispersion of bulk graphitic SiC along the G-M-K-G path (soft modes near the gamma point are numerical artifacts and disappear in sufficiently large supercells with finer grids, see below)

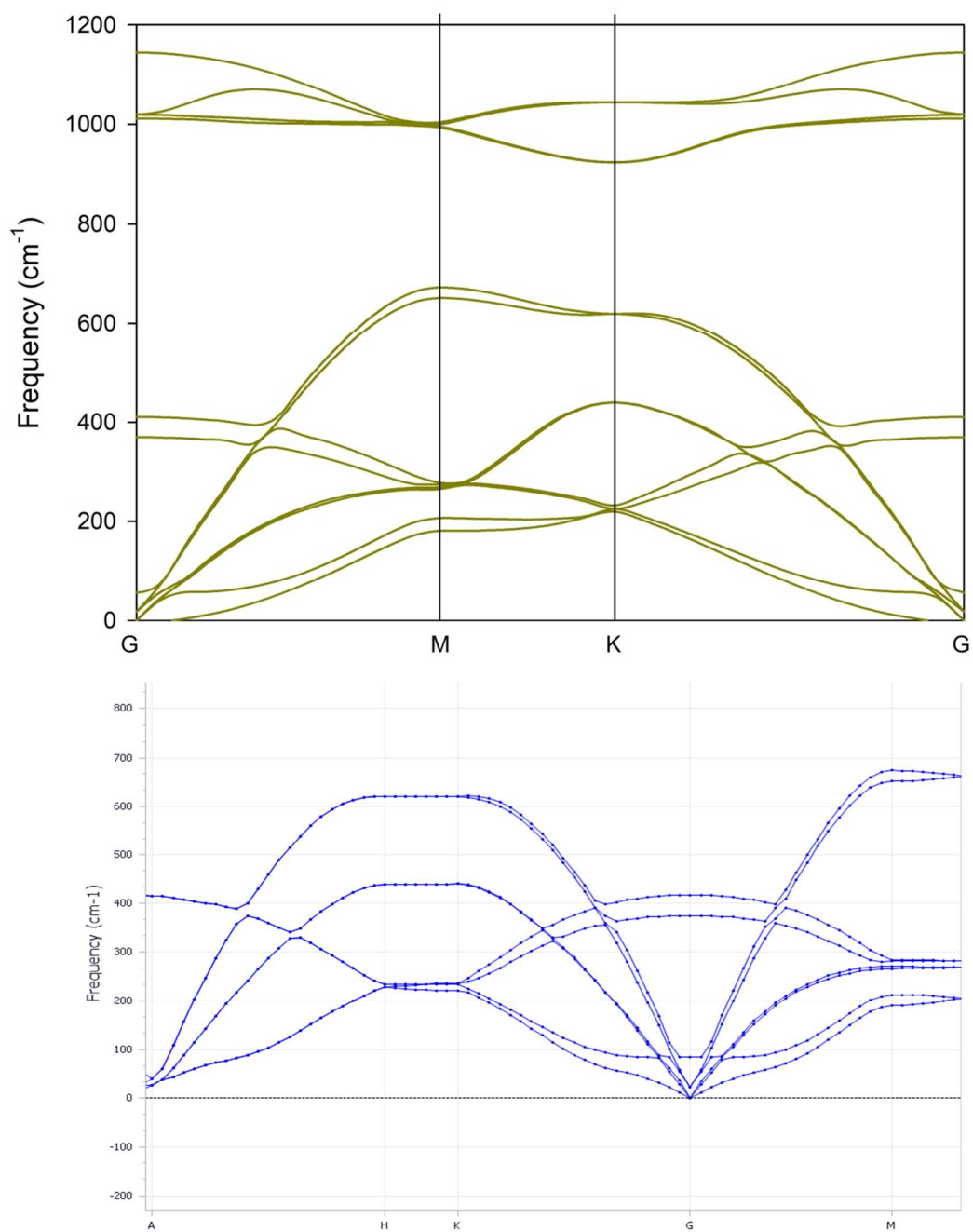


Fig. S6. IR footprint of AB' silagraphite versus that of 3C-SiC

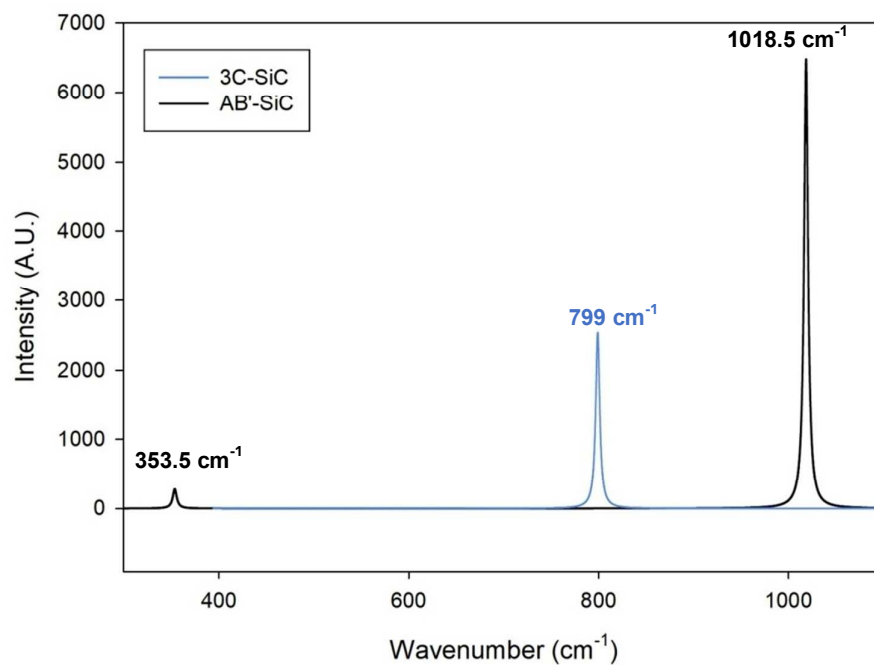


Fig. S7. Density of Phonon States for bilayer and trilayer AA and AB shows how the addition of layers shifts the ultralow frequency acoustic modes (ZA) toward imaginary values (below zero)

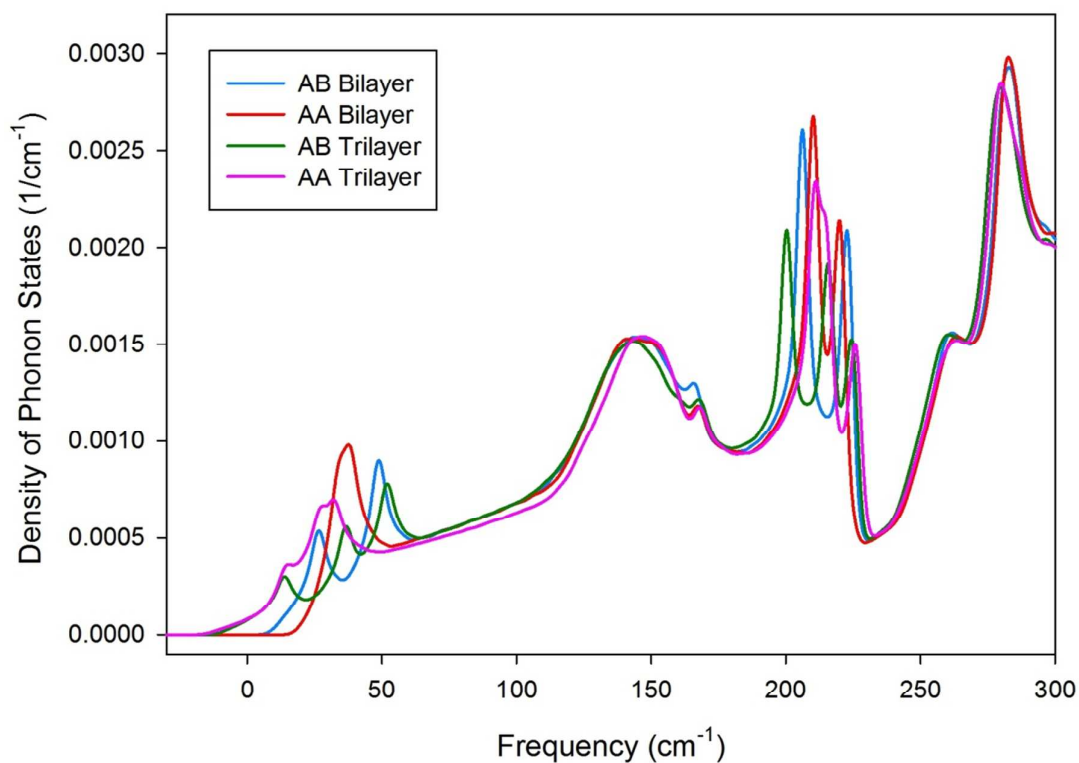


Fig. S8. A close-up of the CBM in monolayer silagraphene

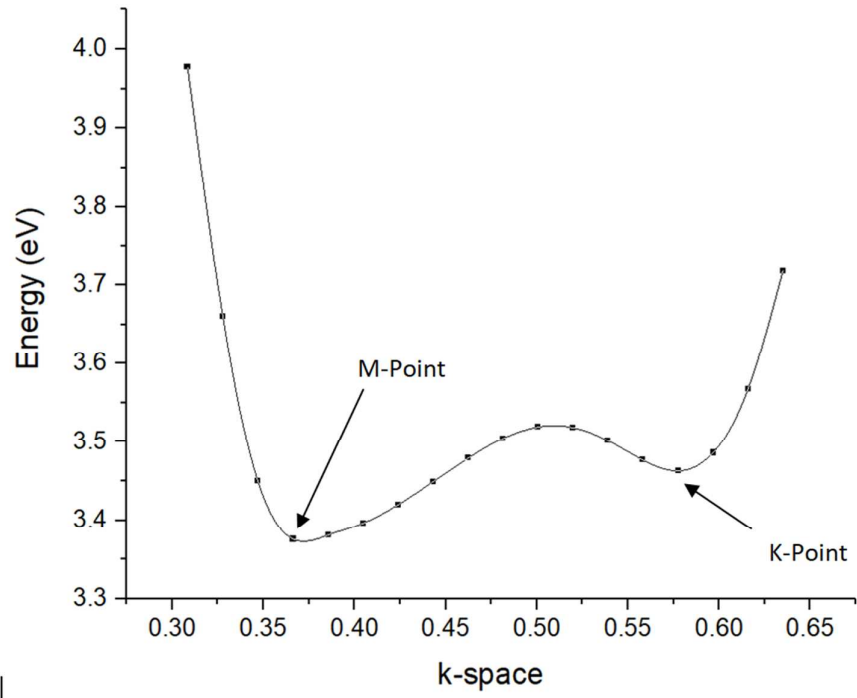


Fig. S9. Band structure of bulk graphitic SiC along the G-M-K-G path shows the indirect and direct gaps more clearly.

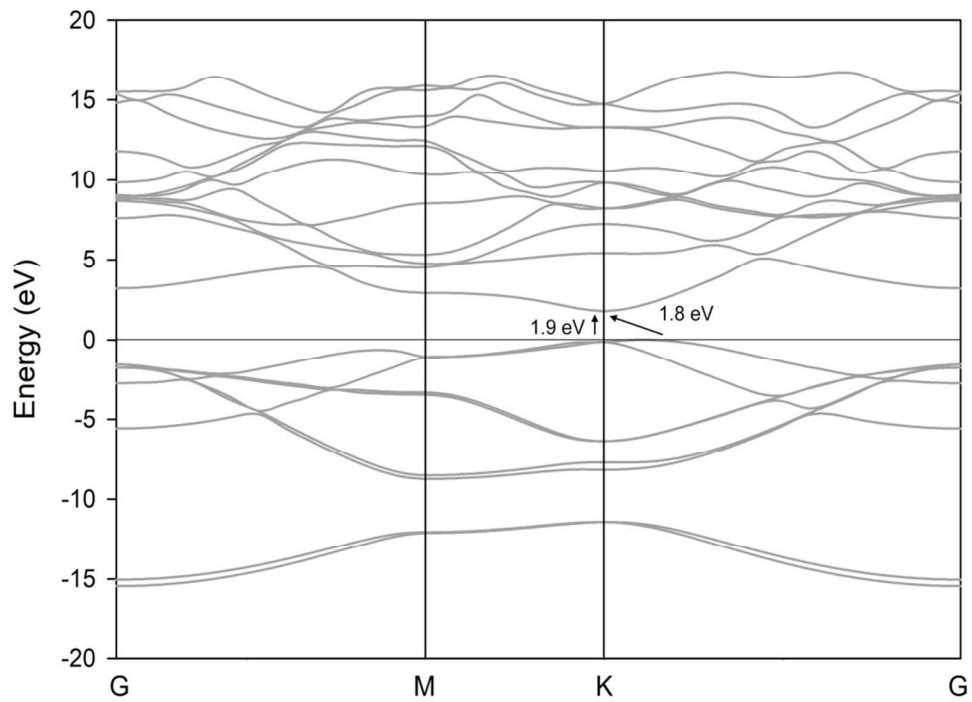


Fig. S10. A series of HRTEM micrographs showing onion-like features that exhibit admixture of several interlayer spacing, but predominantly 3.7 Å. The outlined region shows superposition of two onions.

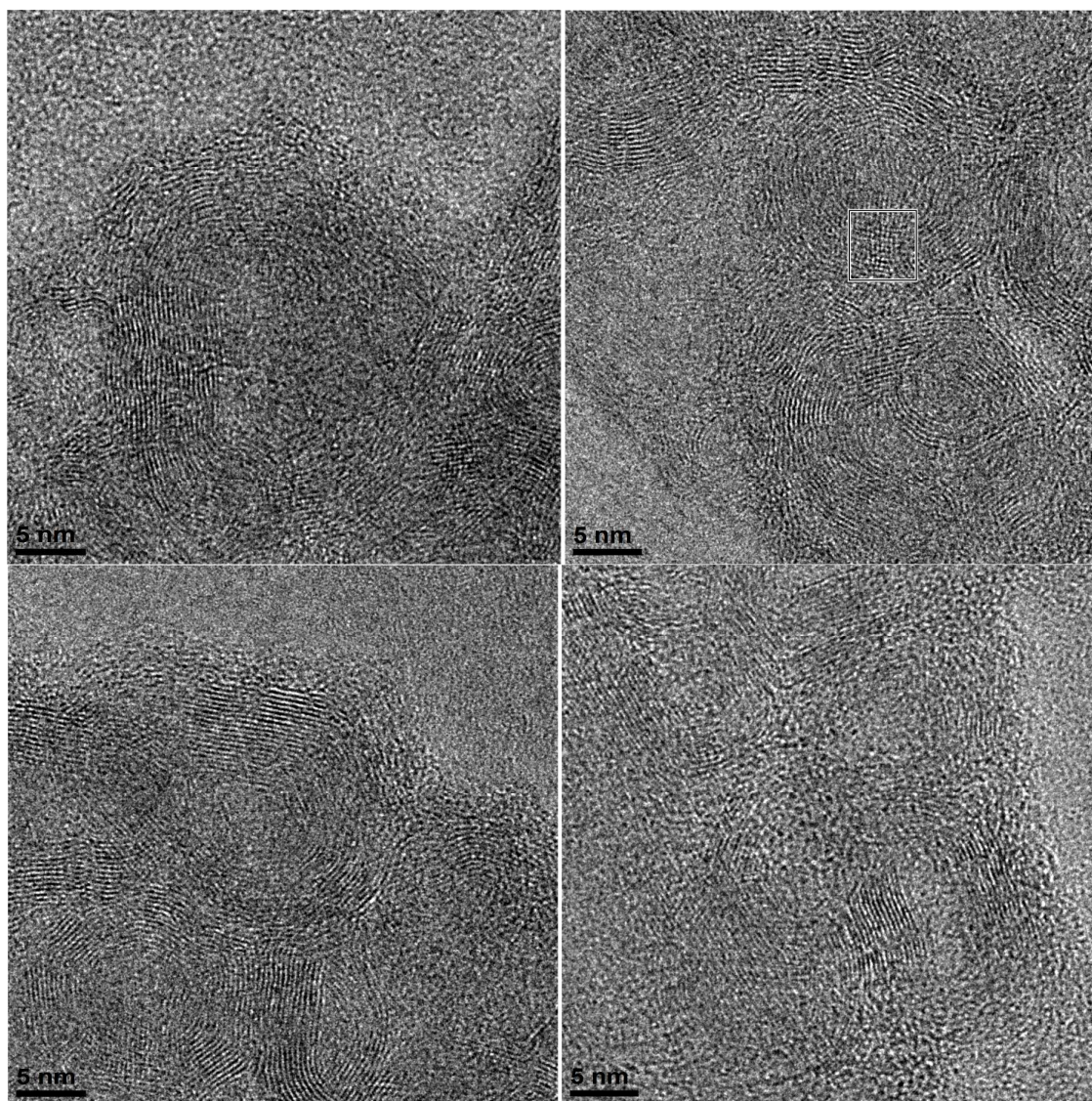


Fig. S11. Line profiles taken from a slightly puckered onion along with its FFT pattern. The scatter plot at the end summarizes the repeating measurements of interlayer spacing

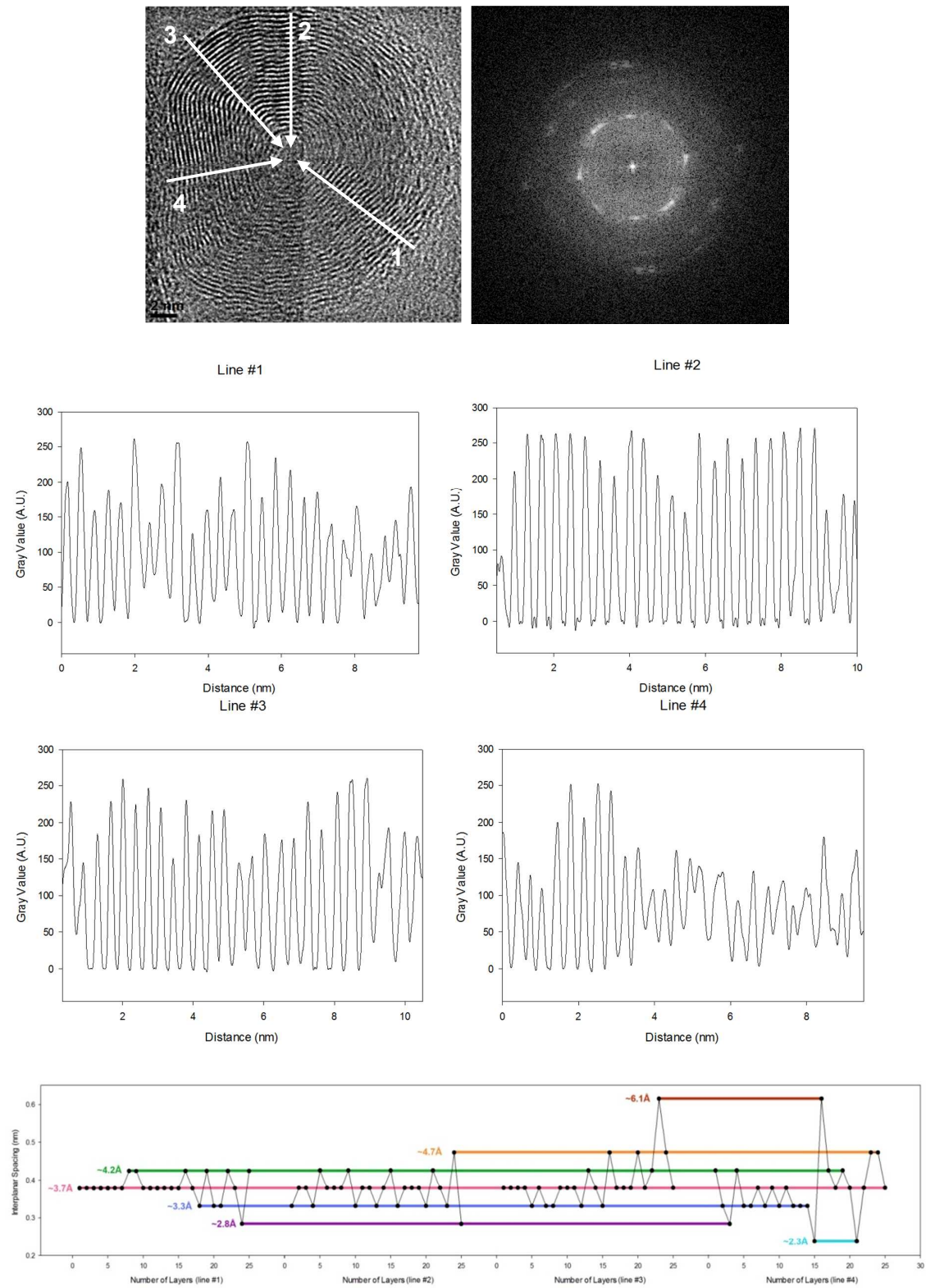


Fig. S12. A pair of HRTEM micrographs showing an onion before (top) and after (bottom) the growing diamond-like core tears it open from within.

