Supplementary information

A superhard and superdense carbon allotrope with all-sp^3 bonded helical chains of five-membered rings

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The crystallographic information file (CIF) for the T-C_{10} crystal structure

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C2    C1     1.585   3_544 S
C2    C1     1.585   4_454 S
C2    C1     1.585   6_446 S
C2    C1     1.585   5_556 S
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To verify the consistency of the results obtained from different calculation methods, we performed geometry optimization and property characterization on T-C_{10} using both CASTEP and VASP. As shown in Table S1, the lattice parameters optimized by CASTEP and VASP are identical, and the corresponding elastic constants demonstrate excellent agreement. Additionally, the band gap of T-C_{10} simulated with CASTEP is 3.31 eV (Fig. S2), which is in close agreement with the 3.34 eV obtained from VASP calculations (Fig. 2e). We also used CASTEP to calculate the stress-strain curves of T-C_{10} along specific crystal orientations (Fig. S3). The tensile strengths of T-C_{10} along the [001] and [100] directions were found to be 132.2 and 26.0 GPa, respectively, with corresponding strains of 0.21 and 0.06, which match the values obtained from VASP calculations.

Table S1. The lattice constants *a*, *b*, and *c* (Å) and elastic constants C_{ij}s (GPa) of T-C_{10} by different calculation methods.

Structure	Methods	Lattice	C_{11}	C_{12}	C_{13}	C_{16}	C_{33}	C_{44}	C_{66}
T-C_{10}	VASP	*a*=*b*=2.78, *c*=7.06	798.1	125.1	115.2	-57.9	1302.1	553.5	482.3
	CASTEP	*a*=*b*=2.78, *c*=7.06	785.3	117.2	108.0	-57.8	1289.6	549.9	475.7

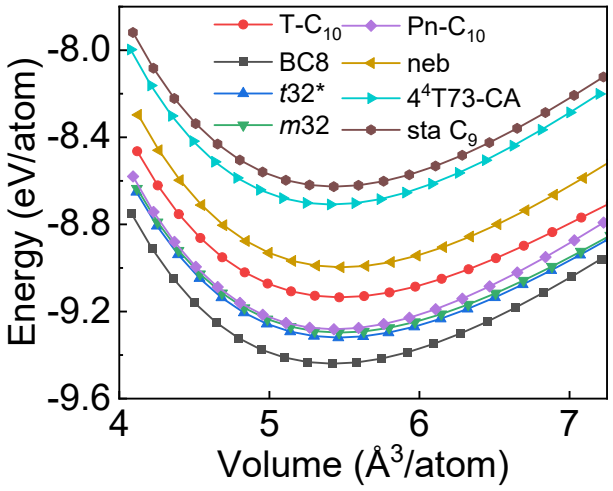

Fig. S1 The total energy as a function of volume per atom for T-C_{10} in comparison with other superhard carbon allotropes.

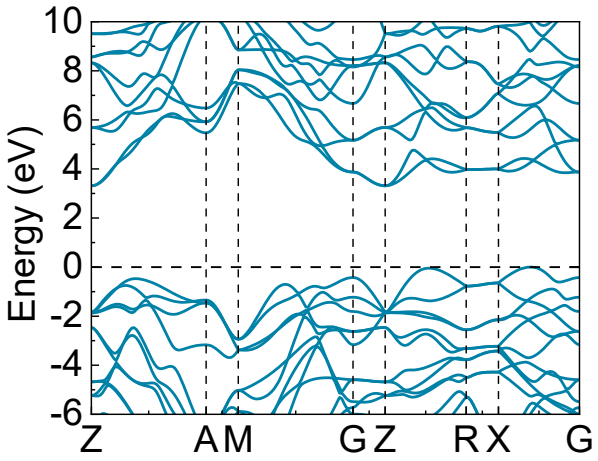

Fig. S2 Electronic band structure of T-C_{10}, calculated using the LDA functional implemented in the CASTEP code. The conduction band minimum (CBM) resides at the Z symmetry point, while the valence band maximum (VBM) emerges between the X and G points. The simulated band gap is 3.31 eV.

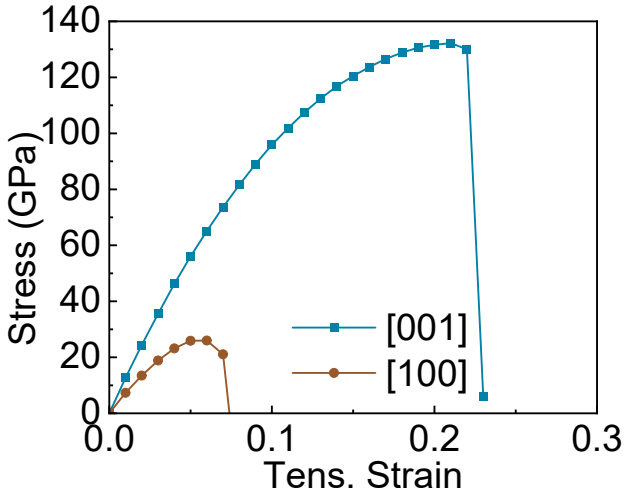

Fig. S3 Strain–stress relationships under the tensile (Tens.) deformations of T-C_{10} along the crystal orientations of [001] and [100], calculated using CASTEP code.