

Fig. S1. Phonon dispersion curves and partial phonon density of states of bcc-C40 carbon at (a) ambient pressure and (b) 150 GPa, denoted by C1 (diatomic carbon), C2 (4-fold helical chains), respectively.

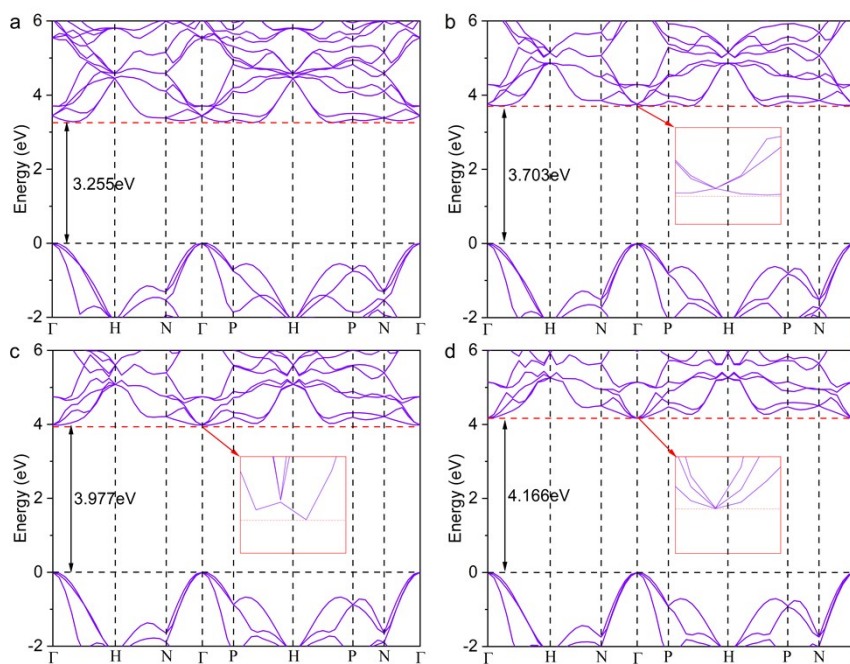


Fig. S2. Band structure with HSE06 method of bcc-C40 carbon at 0 GPa (a), 50 GPa (b), 100 GPa (c) and 150 GPa (d). The illustrations in the (b), (c) and (d) are near the lowest conduction band.

Table S1. Calculated bulk moduli (B , GPa), shear moduli (G , GPa), G/B , Vickers hardness H_V (GPa) based on Chen's¹ (H_V^{Chen} , GPa) and Tian's² model (H_V^{Tian} , GPa), and reference Vickers hardness (H_V^{ref} , GPa) for each of bcc-C40 carbon, C20-T, C96, T-carbon and diamond at ambient pressure.

Structure	B	G	H_V^{Chen}	H_V^{Tian}	H_V^{ref}
bcc-C40	340	343	57.96	88.47	-
C20-T	405	419	68.63	94.48	73.42 ³
C96	270	236	37.72	78.85	-
T-carbon	161	52	4.21	61.94	5.6 ⁴
diamond	451	547	99.44	98.22	98 ⁵

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