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# A new tetragonal superhard metallic carbon allotrope

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## Abstract

A new metallic superhard carbon allotrope  $C_5$  with five carbon atoms per unit cell is theoretically predicted to be stable at ambient pressure through first-principles calculations combined with unbiased swarm structure searching techniques. This novel carbon allotrope consisting of a mixture of  $sp^2$  and  $sp^3$  carbon network exhibits excellent mechanical properties with claimed hardness of 58.5 GPa. Results from our calculated strain-stress relationship reveals that the failure mode of crystal lattice for  $C_5$  is dominated by shear type in the (010)[101] direction with shear stress magnitude of 74.3 GPa. The calculated electronic band structure of  $C_5$  suggests its metallic nature. Detailed analyses of band decomposed charge density show that the metallic nature is contributed by the  $sp^2$  carbon atoms, which form conducting pathways along the  $a$ - and  $b$ -axes.

**Keywords:** superhard metallic carbon; first-principles calculations; mechanical and electronic properties

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