Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIAL

Bottom-up design of carbon allotropes with tunable properties

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Table S1. The detail atomic wyckoff positions of Pco-C_{24}, Pco-C_{24}', Pco-C_{12} and Pco-C_6.

	Method	Atomic wyckoff positions
Pco-C_{24}	LDA	C1 (0.18521, 0.50000, 0.40682) C2 (0.50000, 0.50000, 0.19680)
Pco-C_{24}'	LDA	C1 (0.14583, 0.16935, -0.69879) C2 (0.00000, 0.41605, 0.00000)
Pco-C_{12}	LDA	C1 (0.43218, 0.34449, -0.97228) C2 (0.56805, 0.84841, -0.63951) C3 (0.56552, 0.33803, -0.34914)
Pco-C_6	LDA	C1 (-0.75000, -0.00000, 0.11507) C2 (-0.25000, 0.29504, 0.61729)

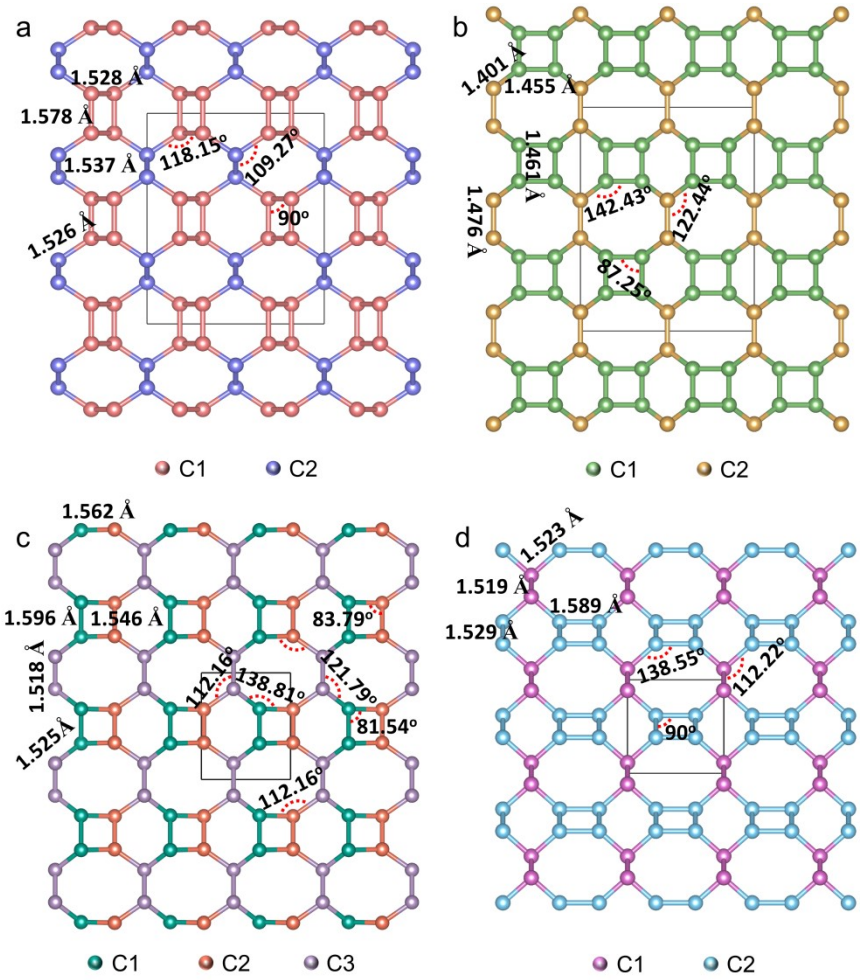

Figure S1. The bond lengths of the neighboring carbon atoms and bond angles of Pco-C_{24} (a), Pco-C_{24}' (b), Pco-C_{12} (c) and Pco-C_6 (d).

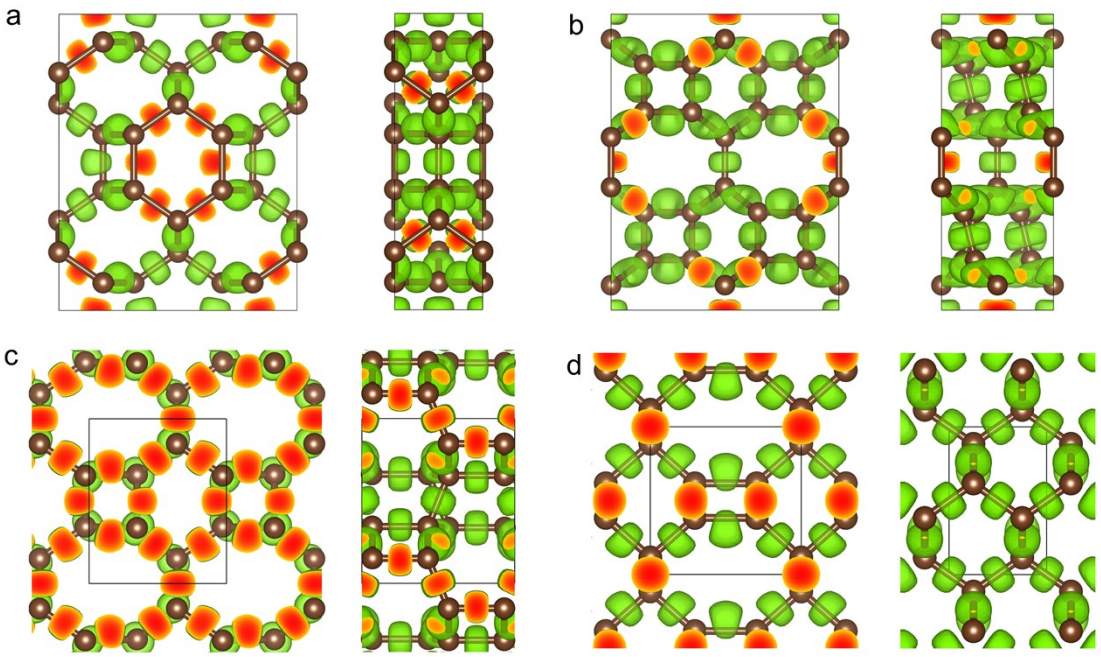

Figure S2. Electron localization function (ELF) of Pco-C_{24} (a), Pco-C_{24}' (b), Pco-C_{12} (c) and Pco-C_6 (d) with an isosurface level set to 0.75.

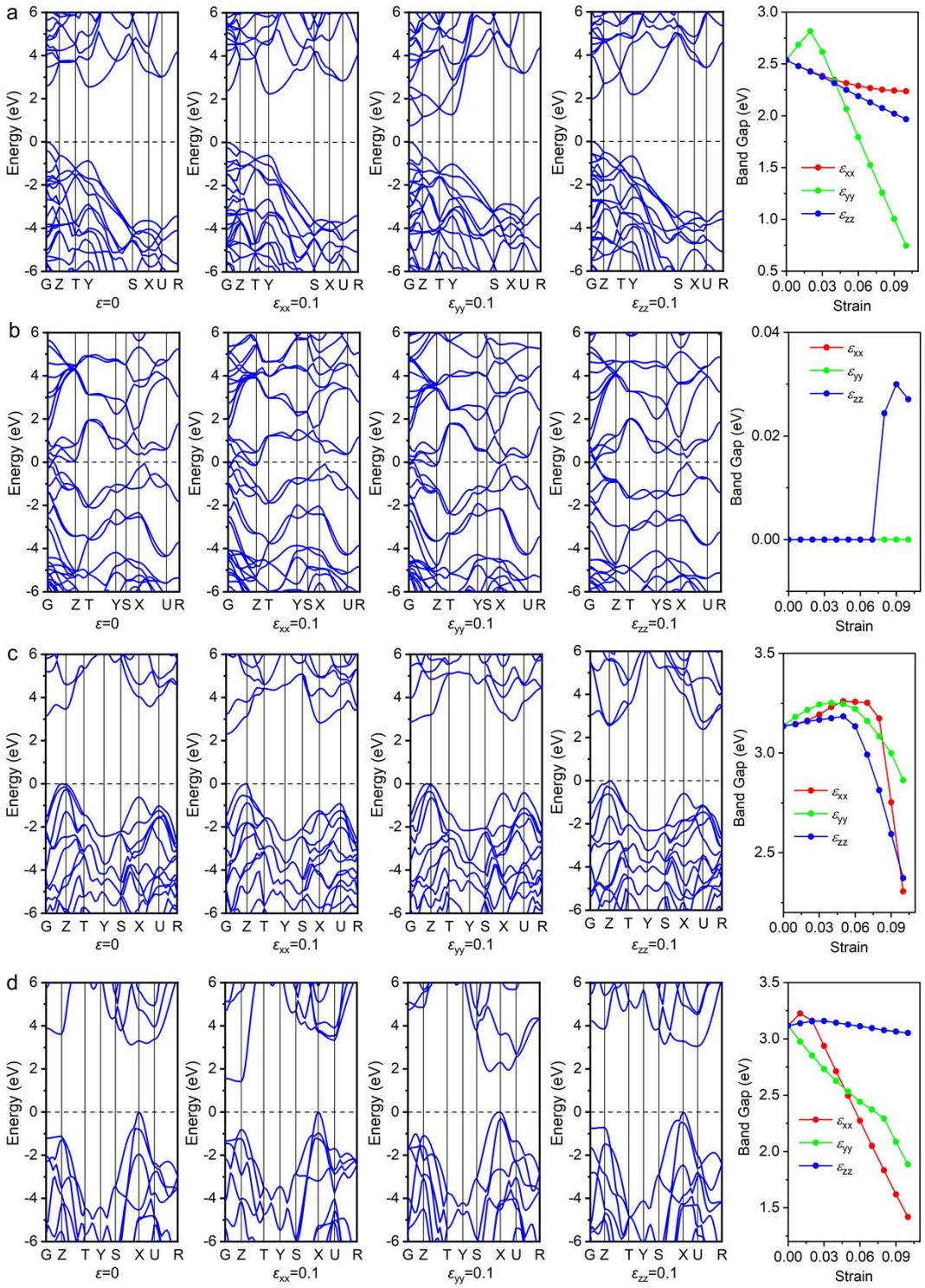

Figure S3. The band structures with uniaxial strain of 0% and 10% applied along the *x*, *y* and *z* directions and the band gap curves with strain. (a) Pco-C_{24}; (b) Pco-C_{24}'; (c) Pco-C_{12}; (d) Pco-C_6.