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

Supplementary materials

Novel carbon allotropes in all-sp^2 bonding networks: Self-assembling design and first-principles calculations

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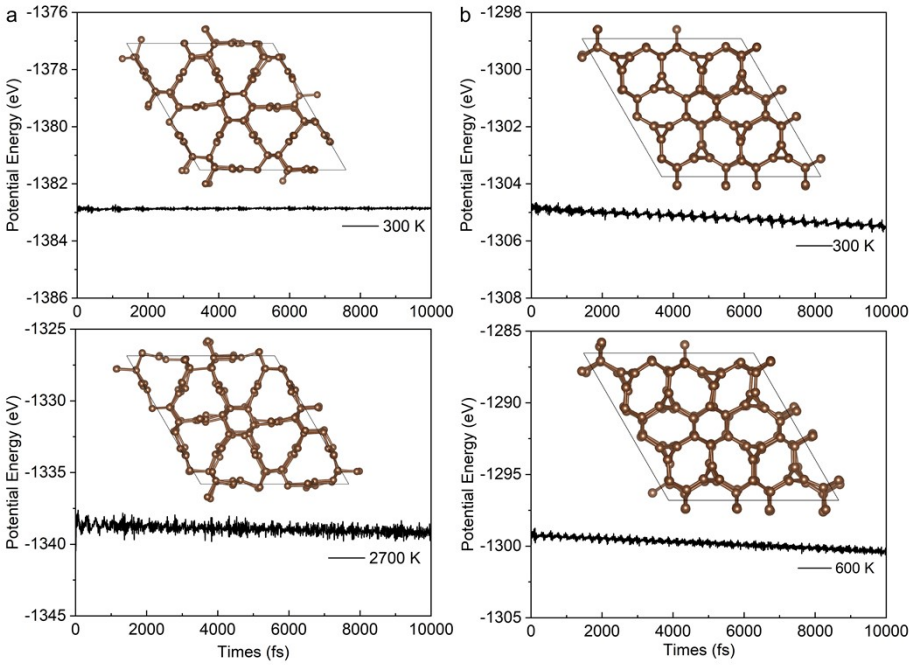

Figure S1. Total potential energy fluctuations of H61-carbon (a) and H62-carbon (b) during the MD simulations. The inset figures show the final structures after the MD simulations at different temperatures.

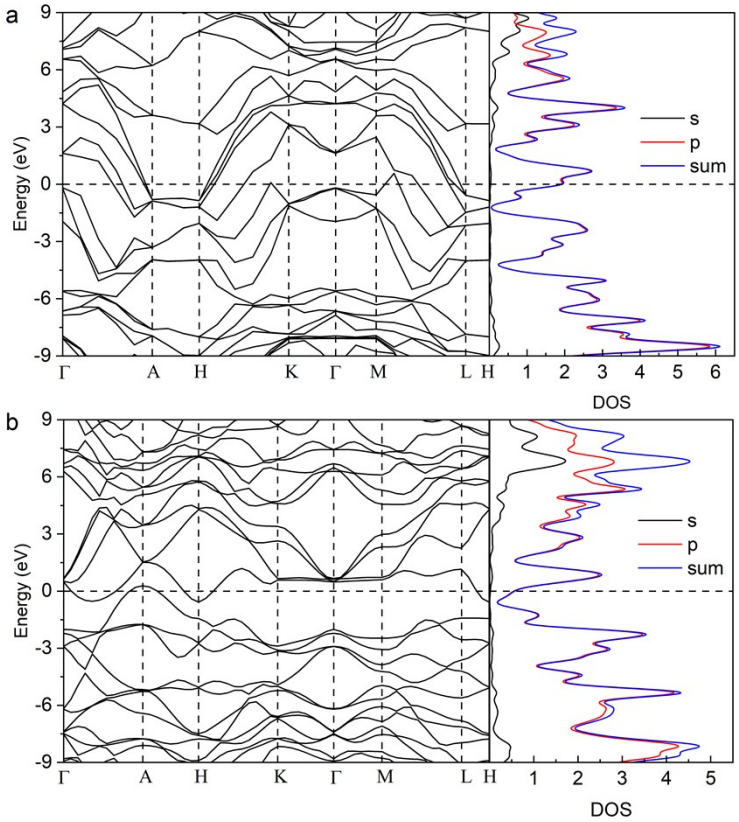

Figure S2. Electronic band structures and the density of states of H61-carbon (a) and H62-carbon (b) at ambient pressure using the HSE06.

Table S1. Calculated coulomb repulsion parameter μ, electron–phonon coupling constant λ, The logarithmic average frequency ω_{log}, and superconducting transition temperature T_C of $H6^1$-carbon and $H6^2$-carbon.

	$H6^1$-carbon			$H6^2$-carbon		
μ	λ	ω_{log}	T_c	λ	ω_{log}	T_c
0.08	0.57176	503.923	12.338	0.47293	771.988	10.182
0.09	0.57176	503.923	11.094	0.47293	771.988	8.760
0.10	0.57176	503.923	9.911	0.47293	771.988	7.452
0.11	0.57176	503.923	8.790	0.47293	771.988	6.260
0.12	0.57176	503.923	7.734	0.47293	771.988	5.184
0.13	0.57176	503.923	6.746	0.47293	771.988	4.225
0.14	0.57176	503.923	5.827	0.47293	771.988	3.382