Supporting Information for "Porosity as a new property control factor in graphene-like 2D allotropes"

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Table S1 Calculated lattice constants, atomic positions of the 1-8 along formation energy edges.

Allotrope		a (Å)	b (Å)	γ (°)	Space group	Atomic positions
12C	1	2.468	2.468	120.000	P6/mmm	C1 (0.333 0.667 0.500) C2 (0.667 0.333 0.500)
	2	4.832	6.706	90.000	Pmma	C1 (0.488 0.714 0.500) C2 (0.250 0.591 0.500) C3 (0.250 0.378 0.500) C4 (0.906 0.080 0.500)
	3	9.119	3.679	90.000	Cmmm	C1 (0.827 0.690 0.500) C2 (0.423 0.500 0.500)
	4	7.084	9.894	90.000	Cmmm	C1 (0.500 0.370 0.500) C2 (0.682 0.572 0.500) C3 (0.808 0.686 0.500) C4 (0.000 0.277 0.500)
	5	19.228	3.909	90.000	Cmmm	C1 (0.149 0.185 0.500) C2 (0.217 0.324 0.500) C3 (0.032 0.500 0.500) C4 (0.897 0.500 0.500)
	6	3.814	10.941	90.000	Pmmm	C1 (0.500 0.702 0.500) C2 (0.500 0.174 0.500) C3 (0.500 0.060 0.500) C4 (0.320 0.500 0.500) C5 (0.186 0.379 0.500)
	7	24.551	3.684	90.000	Cmmm	C1 (0.779 0.190 0.500) C2 (0.186 0.500 0.500) C3 (0.130 0.500 0.500) C4 (0.975 0.500 0.500) C5 (0.079 0.500 0.500)
	8	5.021	9.954	96	P2/m	C1 (0.660 0.943 0.500) C2 (0.974 0.433 0.500) C3 (0.872 0.169 0.500) C4 (0.075 0.691 0.500) C5 (0.376 0.911 0.500) C6 (0.934 0.930 0.500)
14B	1	6.755	5.846	90.000	Cmmm	B1 (0.500 0.500 0.500) B2 (0.748 0.500 0.500) B3 (0.125 0.747 0.500)
	2	6.073	5.093	106.346	P2/m	B1 (0.126 0.2913 500) B2 (0. 137 0.630 0.500) B3 (0.380 0.877 0.500) B4 (0.624 0.460 0.500) B5 (0.125 0.962 0.500)
	3	8.417	2.911	90.000	Cmmm	B1 (0.094 0.500 0.500) B2 (0.705 0.500 0.500)
	4	7.221	4.509	90.000	Pmma	B1 (0.971 0.320 0.500) B2 (0.882 0.972 0.500) B3 (0.250 0.742 0.500)
	5	8.684	7.452	113.372	Pm	B1 (0.662 0.147 0.500) B2 (0.967 0.528 0.500) B3 (0.982 0.146 0.500) B4 (0.862 0.288 0.500) B5 (0.563 0.915 0.500) B6 (0.317 0.163 0.500) B7 (0.012 0.764 0.500) B8 (0.771 0.004 0.500) B9 (0.168 0.666 0.500) B10 (0.083 0.403 0.500) B11 (0.201 0.283 0.500) B12 (0.451 0.056 0.500) B13 (0.238 0.915 0.500) B14 (0.901 0.900 0.500) B15 (0.367 0.798 0.500) B16 (0.109 0.029 0.500)
	6	7.301	7.301	120	Pm	B1 (0.677 0.923 0.500) B2 (0.330 0.701 0.500) B3 (0.617 0.315 0.500) B4 (0.862 0.885 0.500) B5 (0.384 0.516 0.500) B6 (0.948 0.722 0.500) B7 (0.771 0.522 0.500) B8 (0.979 0.512 0.500) B9 (0.176 0.483 0.500) B10 (0.539 0.713 0.500) B11 (0.141 0.709 0.500) B12 (0.010 0.298 0.500) B13 (0.849 0.102 0.500) B14 (0.645 0.118 0.500) B15 (0.569 0.503 0.500) B16 (0.819 0.316 0.500)
	7	8.2390	7.245	68.723	P2/m	B1 (0.803 0.361 0.500) B2 (0.585 0.403 0.500)

						B3 (0.280 0.816 0.500) B4 (0.045 0.284 0.500) B5 (0.161 0.051 0.500) B6 (0.897 0.519 0.500) B7 (0.940 0.119 0.500)
	8	8.163	7.354	114.891	Pm	B1 (0.883 0.865 0.500) B2 (0.087 0.895 0.500) B3 (0.691 0.833 0.500) B4 (0.270 0.299 0.500) B5 (0.935 0.466 0.500) B6 (0.166 0.499 0.500) B7 (0.019 0.686 0.500) B8 (0.296 0.908 0.500) B9 (0.175 0.101 0.500) B10 (0.519 0.948 0.500) B11 (0.222 0.711 0.500) B12 (0.069 0.305 0.500) B13 (0.816 0.651 0.500) B14 (0.382 0.110 0.500)
8B8C	1	5.463	4.333	101.850	P2/m	B1 (0.107 0.372 0.500) B2 (0.868 0.034 0.500) C1 (0.610 0.114 0.500) C2 (0.614 0.444 0.500)
	2	9.517	5.053	90.000	Cmmm	B1 (0.154 0.763 0.500) C1 (0.232 0.500 0.500) C2 (0.000 0.138 0.500)
	3	6.365	7.887	96.709	Pm	B1 (0.308 0.533 0.500) B2 (0.873 0.462 0.500) B3 (0.510 0.250 0.500) B4 (0.557 0.886 0.500) B5 (0.872 0.141 0.500) B6 (0.306 0.969 0.500) B7 (0.540 0.643 0.500) B8 (0.340 0.762 0.500) C1 (0.128 0.824 0.500) C2 (0.732 0.289 0.500) C3 (0.782 0.636 0.500) C4 (0.108 0.418 0.500) C5 (0.106 0.236 0.500) C6 (0.788 0.950 0.500) C7 (0.906 0.802 0.500) C8 (0.296 0.162 0.500)
	4	7.785	5.097	83	Pm	B1 (0.235 0.683 0.500) B2 (0.336 0.397 0.500) B3 (0.853 0.149 0.500) B4 (0.083 0.550 0.500) B5 (0.067 0.841 0.500) B6 (0.615 0.340 0.500) B7 (0.408 0.077 0.500) B8 (0.802 0.623 0.500) C1 (0.244 0.164 0.500) C2 (0.822 0.878 0.500) C3 (0.014 0.114 0.500) C4 (0.482 0.285 0.500) C5 (0.751 0.381 0.500) C6 (0.302 0.917 0.500) C7 (0.940 0.701 0.500) C8 (0.106 0.271 0.500)
	5	6.575	6.410	82	Pm	B1 (0.372 0.686 0.500) B2 (0.514 0.075 0.500) B3 (0.975 0.054 0.500) B4 (0.185 0.680 0.500) B5 (0.841 0.954 0.500) B6 (0.293 0.157 0.500) B7 (0.853 0.301 0.500) B8 (0.726 0.206 0.500) C1 (0.081 0.521 0.500) C2 (0.875 0.622 0.500) C3 (0.617 0.172 0.500) C4 (0.294 0.482 0.500) C5 (0.082 0.206 0.500) C6 (0.182 0.021 0.500) C7 (0.409 0.970 0.500) C8 (0.983 0.705 0.500)
	6	22.940	3.879	90.000	Amm2	B1 (0.217 0.822 0.500) B2 (0.387 0.990 0.500) B3 (0.500 0.262 0.500) B4 (0.500 0.737 0.500) C1 (0.322 0.994 0.500) C2 (0.216 0.214 0.500) C3 (0.552 0.000 0.500)
	7	4.528	10.746	90.000	Pmm2	B1(0.191 0.948 0.500) B2(0.189 0.215 0.500) B3(0.000 0.462 0.500) B4(0.000 0.081 0.500) C1(0.000 0.834 0.500) C2(0.000 0.710 0.500)

						C3(0.000 0.330 0.500) C4(0.000 0.592 0.500) C5(0.500 0.016 0.500) C6(0.500 0.148 0.500)
	8	7.128	7.406	106.936	P2/m	B1 (0.237 0.367 0.500) B2 (0.968 0.598 0.500) B3 (0.799 0.390 0.500) C1 (0.521 0.087 0.500) C2 (0.419 0.718 0.500) C3 (0.548 0.602 0.500)

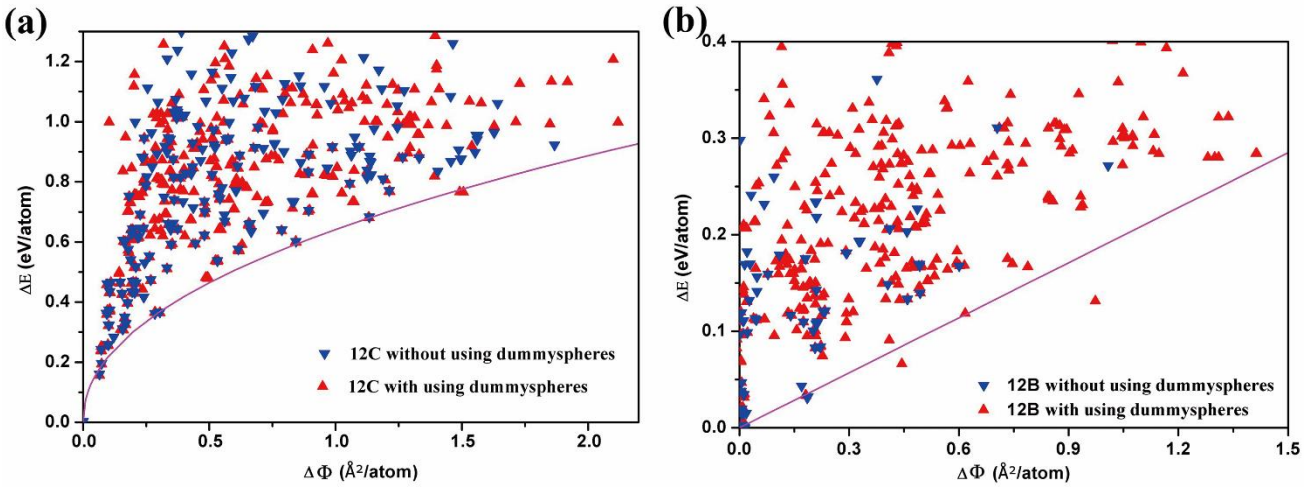

Figure S1 Search results with and without using dummy spheres, 12 carbon atoms per unit (a), 12 boron atoms per unit (b). The 720 structures were used in both search, but there are 705 and 483 valid data for 12 carbon and 12 boron atoms per unit with using dummy spheres, and there are 630 and 347 valid data without using dummy spheres (other structures didn't keep the two dimension during the structure optimization).

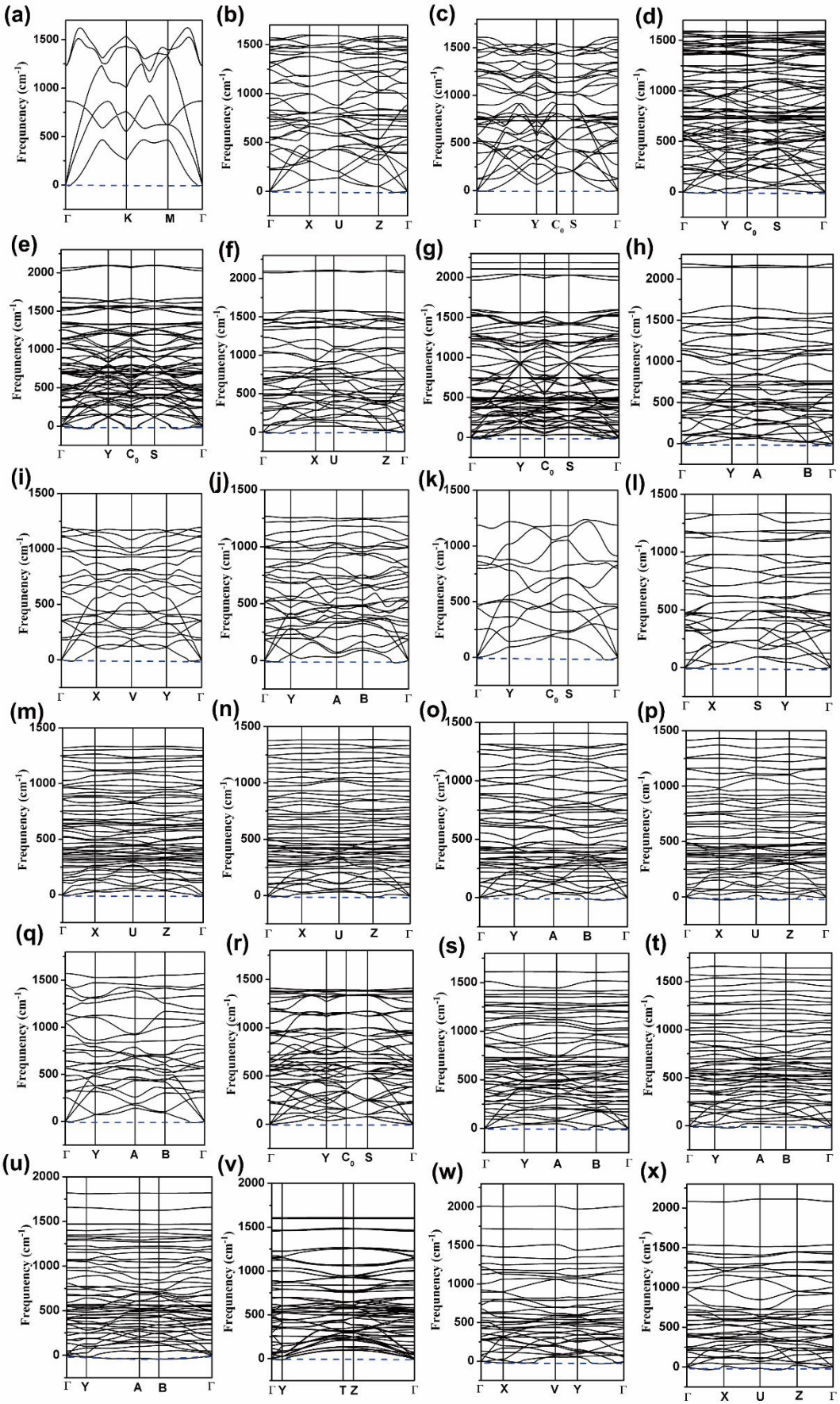

Figure S2 (a)-(h) the phonon spectra of str-1 to str-8 from 12C per unit. (i)-(p) the phonon spectra of str-1 to str-8 from 14B per unit. (q)-(x) the phonon spectra of str-1 to str-8 from 8B8C per unit. The high symmetric points are got from online tool seek-path (from www.materialscloud.org).

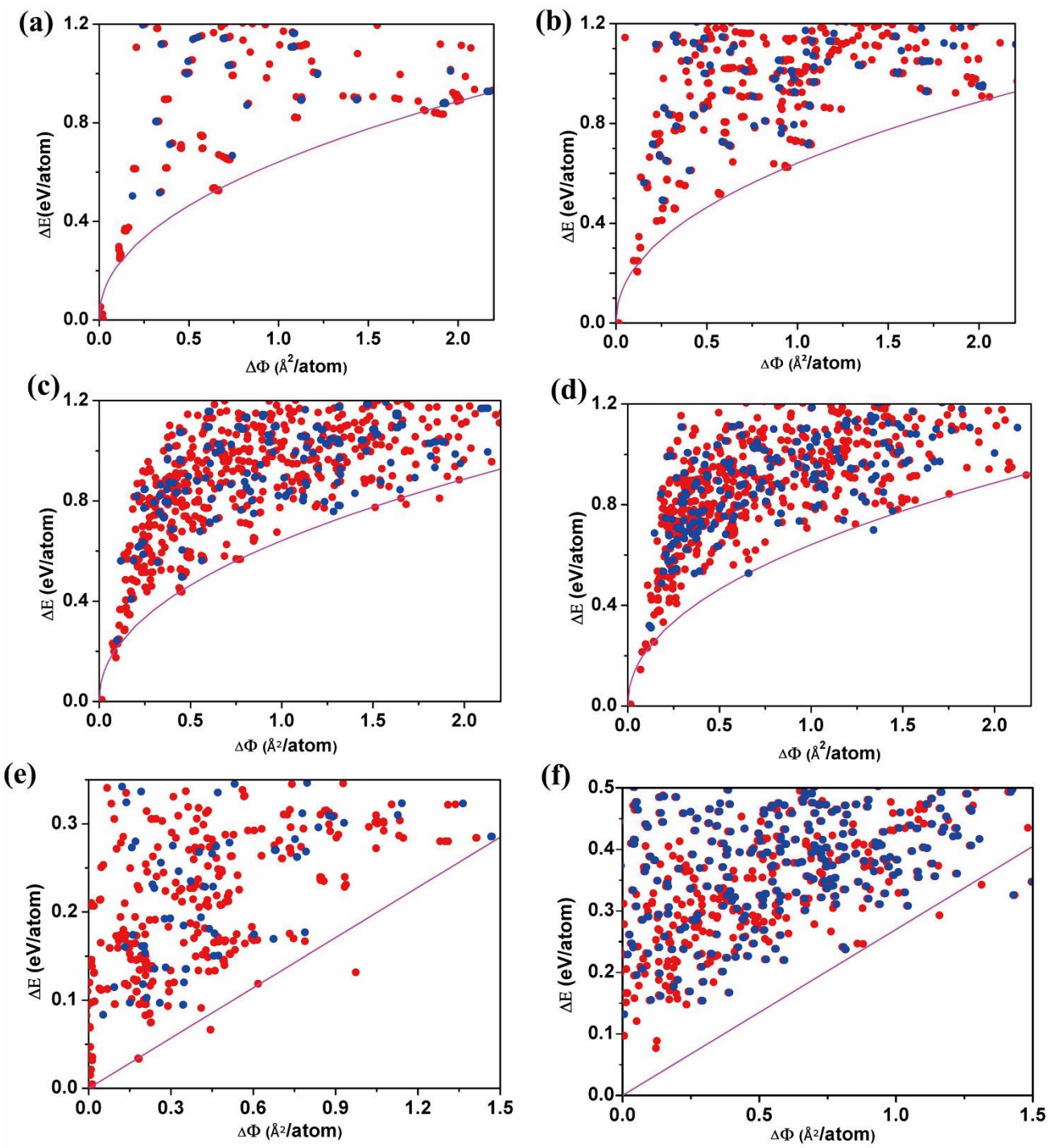

Figure S3 The distribution between energies and atomic porosities for 8 carbon atoms per unit (a), 10 carbon atoms per unit (b), 14 carbon atoms per unit (c), 16 carbon atoms per unit (d), 12 boron atoms per unit (e) and 6 boron atoms 6 carbon atoms per unit(f), respectively. The red and blue dots show the allotropes that are metallic and semiconducting, respectively.

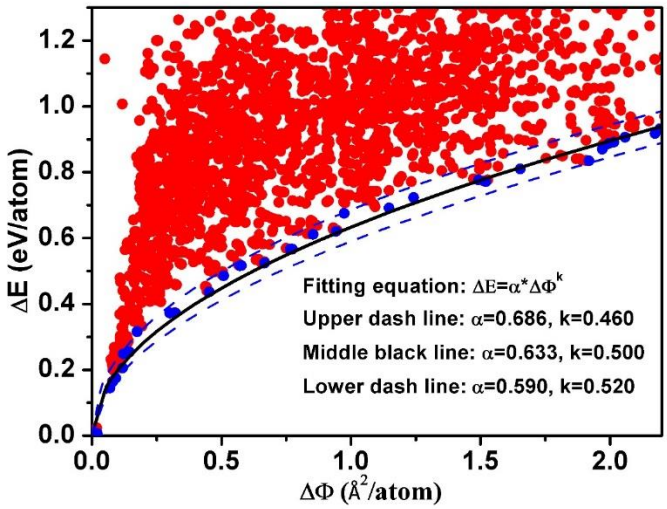

Figure S4 Plotting 3324 structure points of all searches from 8 to 16 carbon atoms per unit. From the fitted value, k varies in a range from 0.46 to 0.52 with an optimal value of 0.5. α changes from 0.686 to 0.590, the best-fitted k value becomes 0.5.

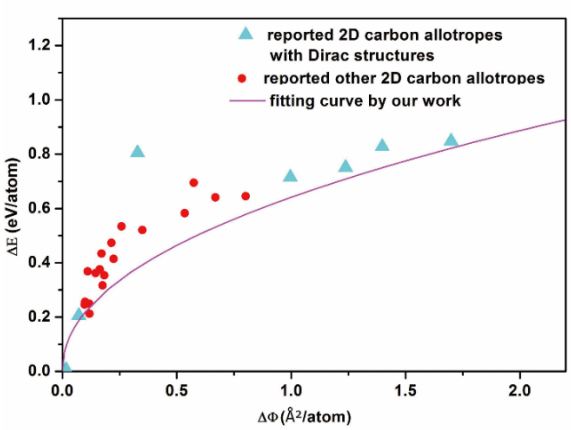

Figure S5 The distribution between energies and atomic porosities for already reported carbon allotropes. Green triangles: structures with Dirac cones, red spheres: others; magenta curve was fitting by our works.

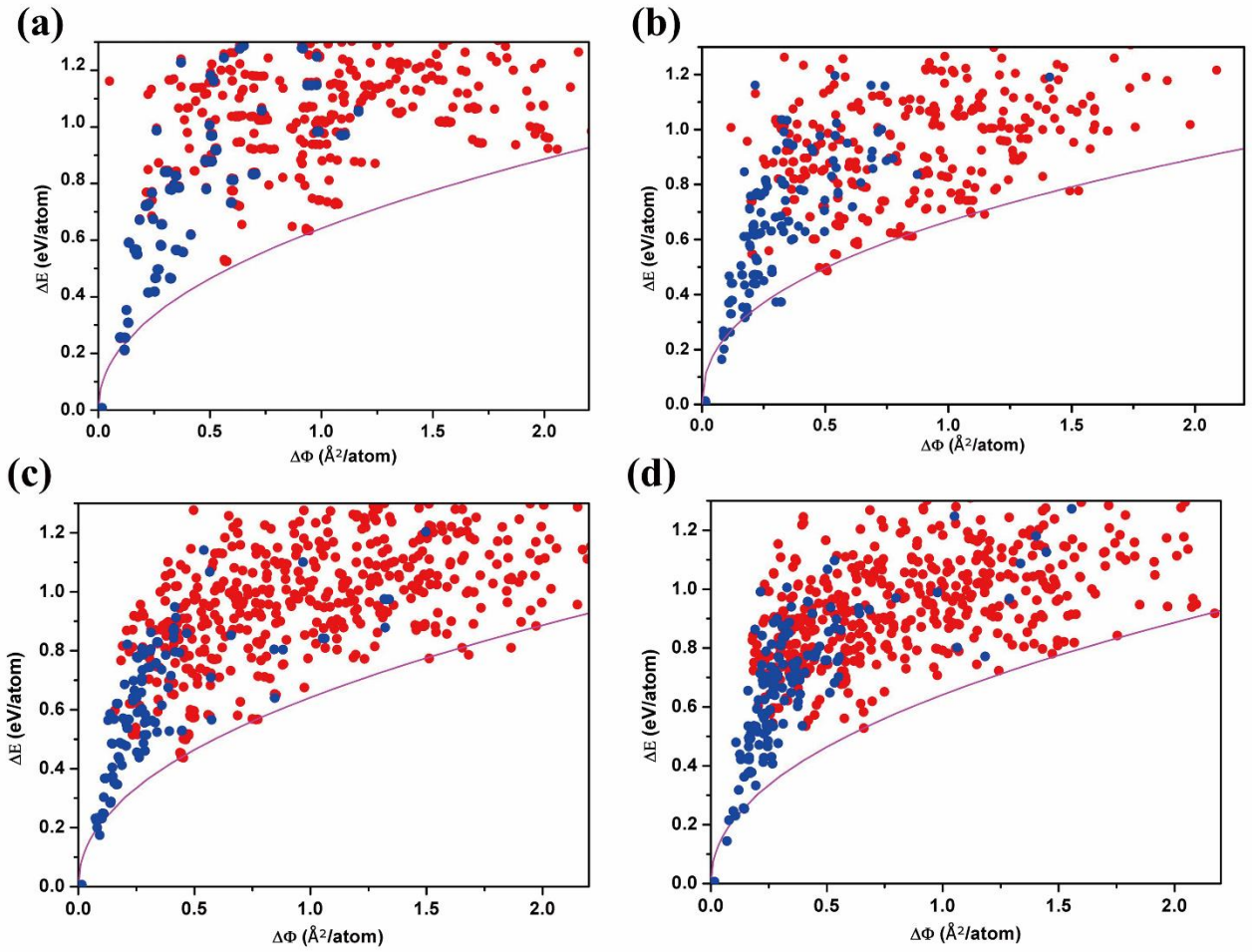

Figure S6 The distribution of total sp^2 and sp^2+sp allotropes with 10 carbon atoms per unit (a),12 carbon atoms per unit(b), 14 carbon atoms per unit (c), 16 carbon atoms per unit (d). Blue sphere: total sp^2 hybridization; red sphere: hybridization style with sp^2 and sp; magenta line: the asymptotic line was fitting by our works.

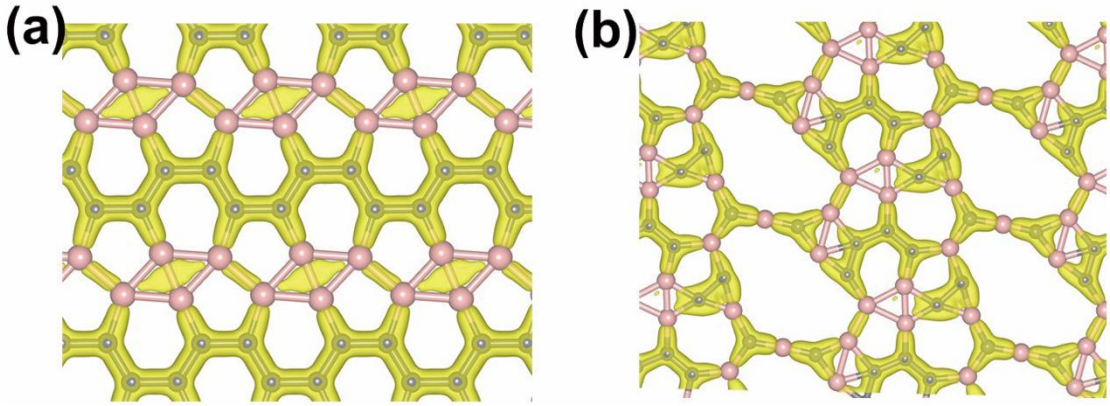

Figure S7 The charge difference for 8B8C (a) structure 1 (metal) and (b) structure 4 (semiconductor), respectively. The isosurface is 0.04 e/Å.

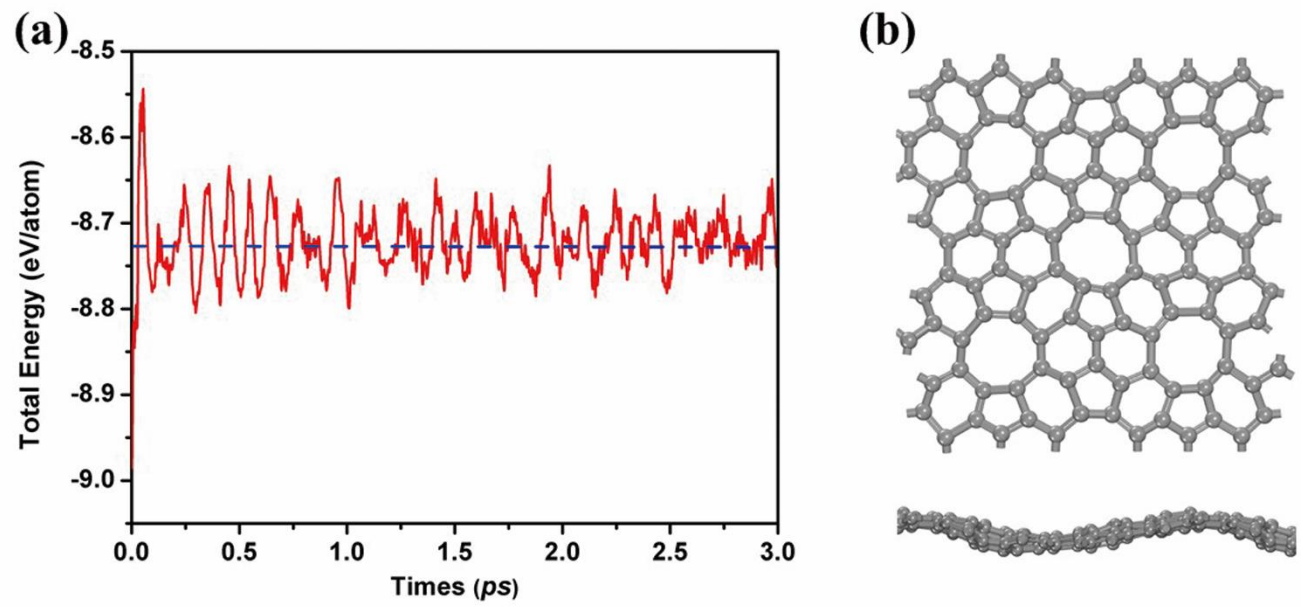

Figure S8 (a) Evolution of total energy as a function of the AIMD simulation step of *Cmmm*-graphene at 2000K; (b) a snapshot of the equilibrium structure of *Cmmm*-graphene after 3 *ps* MD simulation at 2000 K.