Supplemental Material for "(DSF)n-graphene: carbon semimetal with double stacking faults"

Juan Wei[a], Weixiang Kong[a], Xiaoliang Xiao[a], Wangping Xu[b], Rui Wang[a], Li-Yong Gan[a], Jing Fan[c], and Xiaozhi Wu[a,*]

[a]Institute for Structure and Function and Department of Physics, Chongqing University, Chongqing 401331, P. R. China

[b]Hunan Institute of Advanced Sensing and Information Technology, Xiangtan University, Xiangtan, Hunan 411105, P. R. China

[c]Center for Computational Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, P. R. China

Method and computational details

The first-principles calculations were carried out using the density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP)[1,2]. The generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerh (PBE)[3] was adopted for the exchange-correlation functional. The electron-ion interaction was designated by projector augmented wave(PAW) methods potentials[4]. Heyd−Scuseria−Ernzerhof (HSE06) function was used to predict more accurate electronic structure[5]. The energy cutoff employed for plane wave expansion of electron wave-function was set to 520 eV. The convergence criterion of total energy was set to be 1×10^{-6}eV and the thickness of the slab model was set to be larger than 16Å to avoid specious interaction between adjacent atom layers. Geometry optimization was executed until the remanent Hellmann-Feynman forces on the ions were less than 0.01 eV/Å. The Brillouin zone (BZ) of (DSF)$_3$-graphene and (DSF)$_4$-graphene were performed by using $3\times11\times1$ and $3\times13\times1$ Monkhorst-Pack sampling scheme k-point mesh[6], and the dynamic stability of new structures has been examined by the phonon calculations and finite temperature molecular dynamics. Edge states were presented using the iterative Greens method[7] as implemented in the WANNIERTOOLS package.[8] We built the tight-binding (TB) Hamiltonian using

maximally localized Wannier functions (MLWF) methods by using the WANNIER90 package.[9,10]

Table. S1 The corresponding total energies(E_f) and planar atomic density of the newly discovered and previously proposed carbon allotropes relative to graphene.

	E_f (eV/atom)	ρ (atom/Å²)		E_f (eV/atom)	ρ (atom/Å²)
graphene	0	0.379	$(DSF)_1$-graphene	0.4322	0.3528
graphyne	0.640	0.292	$(DSF)_2$-graphene	0.3409	0.3588
BPC	0.630	0.304	$(DSF)_3$-graphene	0.2806	0.3631
T-graphene	0.518	0.336	$(DSF)_4$-graphene	0.2367	0.3659
New-C	0.469	0.353	$(DSF)_5$-graphene	0.2049	0.3678
New-W	0.373	0.358	$(DSF)_6$-graphene	0.1802	0.3693
Hopgraphene	0.25	0.361	$(DSF)_7$-graphene	0.1611	0.3704
δ-graphene	0.262	0.364	$(DSF)_8$-graphene	0.1453	0.3713
Phagraphene	0.19	0.370	$(DSF)_9$-graphene	0.1325	0.3720
ψ-graphene	0.159	0.369	$(DSF)_{10}$-graphene	0.1220	0.3726
SW graphene	0.149	0.372	$(DSF)_{11}$-graphene	0.1129	0.3732
SW40	0.13	0.372	$(DSF)_{12}$-graphene	0.1048	0.3735
			$(DSF)_{13}$-graphene	0.0983	0.3740
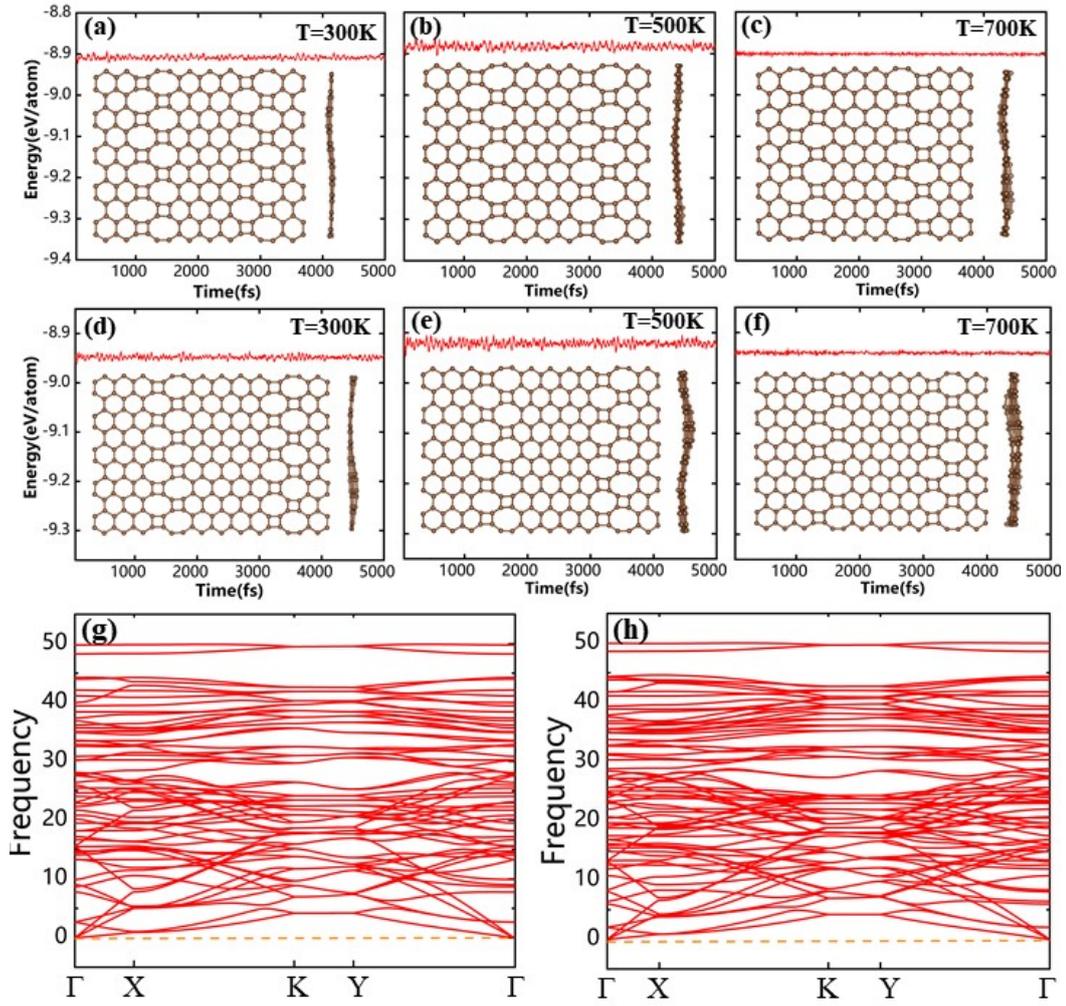
Fig. S1 The molecular dynamics simulations under 300K (500 K and 700 K) and phonon dispersion, (a), (b) and (c) are (DSF)$_3$-graphene, (d), (e) and (f) are (DSF)$_4$-graphene, where (g) and (f) are the phonon spectrums of (DFS)$_3$-graphene and (DSF)$_4$-graphene, respectively.
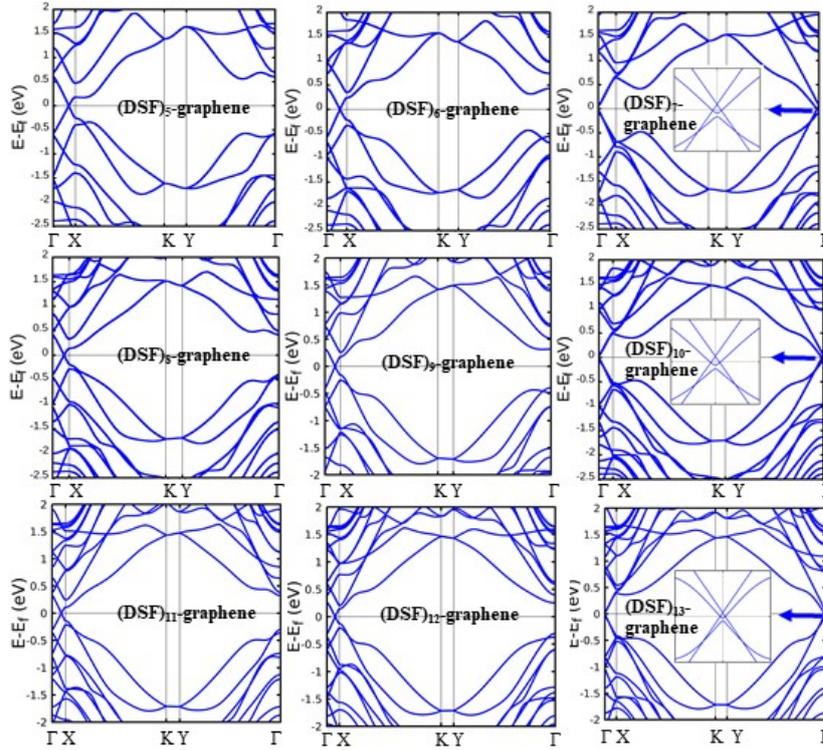
Fig. S2 The band structures of newly discovered carbon allotropes of $(DSF)_n$-graphene, where n increases from 5 to 13. The band structures near the Dirac cones of $(DSF)_7$-graphene, $(DSF)_{10}$-graphene and $((DSF)_{13}$-graphene are enlarged.
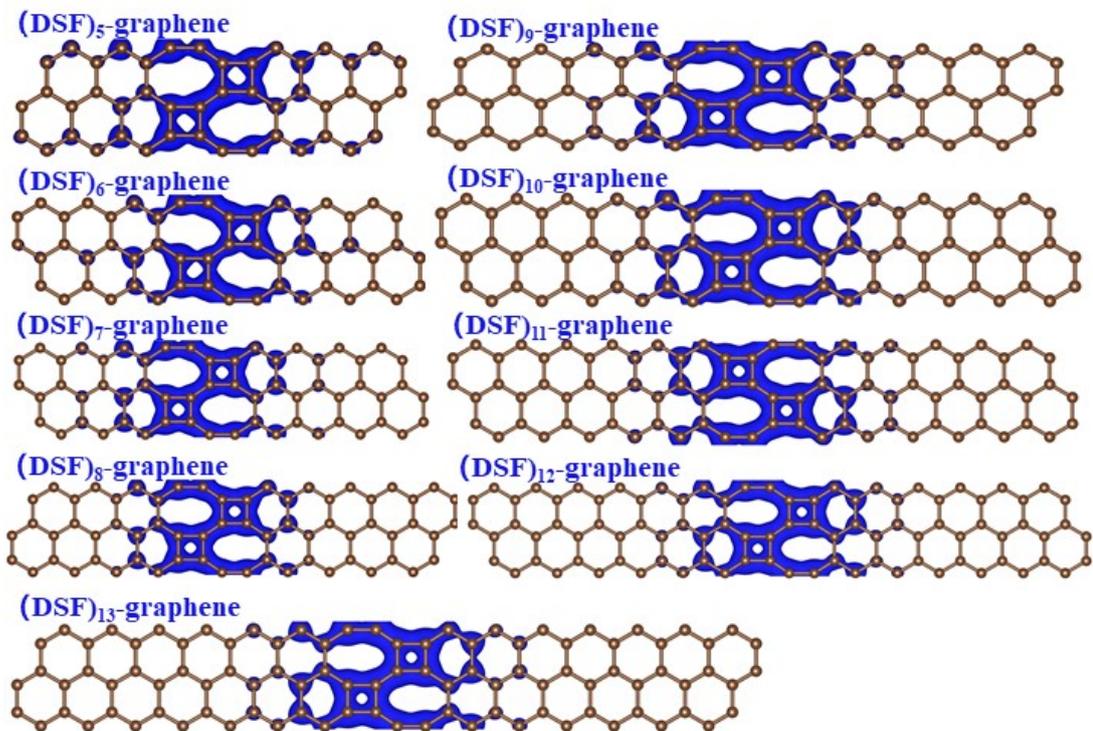
Fig. S3 The corresponding charge in the proximity of Dirac cone is major distributed at the grain boundary along the armchair direction.

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