Supplementary materials for

Newly discovered graphyne allotrope with rare and robust Dirac node loop

Pinlan Yan, Tao Ouyang[a)], Chaoyu He[a)], Jin Li[a)], Chunxiao Zhang, Chao Tang, and Jianxin Zhong

Hunan Key Laboratory for Micro-Nano Energy Materials and Device, Xiangtan University, Xiangtan 411105, Hunan, China

School of Physics and Optoelectronics, Xiangtan University, Xiangtan 411105, Hunan, China

I. The possible synthetic route for 123-E8Y24-1

As shwon in step1, the intramolecular cross-coupling reactions of dimethylmaleic acid ($C_6H_8O_4$) will lead to the formation of compound (1A). Through catalyzing with appropriated acetylene unit, the compound (1A) could be treated to the small flakes of 123-E8Y24-1 (compound (2A)) as presented in step2. Such small flake may serve as the starting material for the synthesis of 123-E8Y24-1 by using promising metal catalyzed cross-coupling reactions, alkyne metathesis and templated synthesis techniques.

[a)]Authors to whom correspondence should be addressed. Electronic addresses: ouyangtao@xtu.edu.cn, hechaoyu@xtu.edu.cn, and lijin@xtu.edu.cn

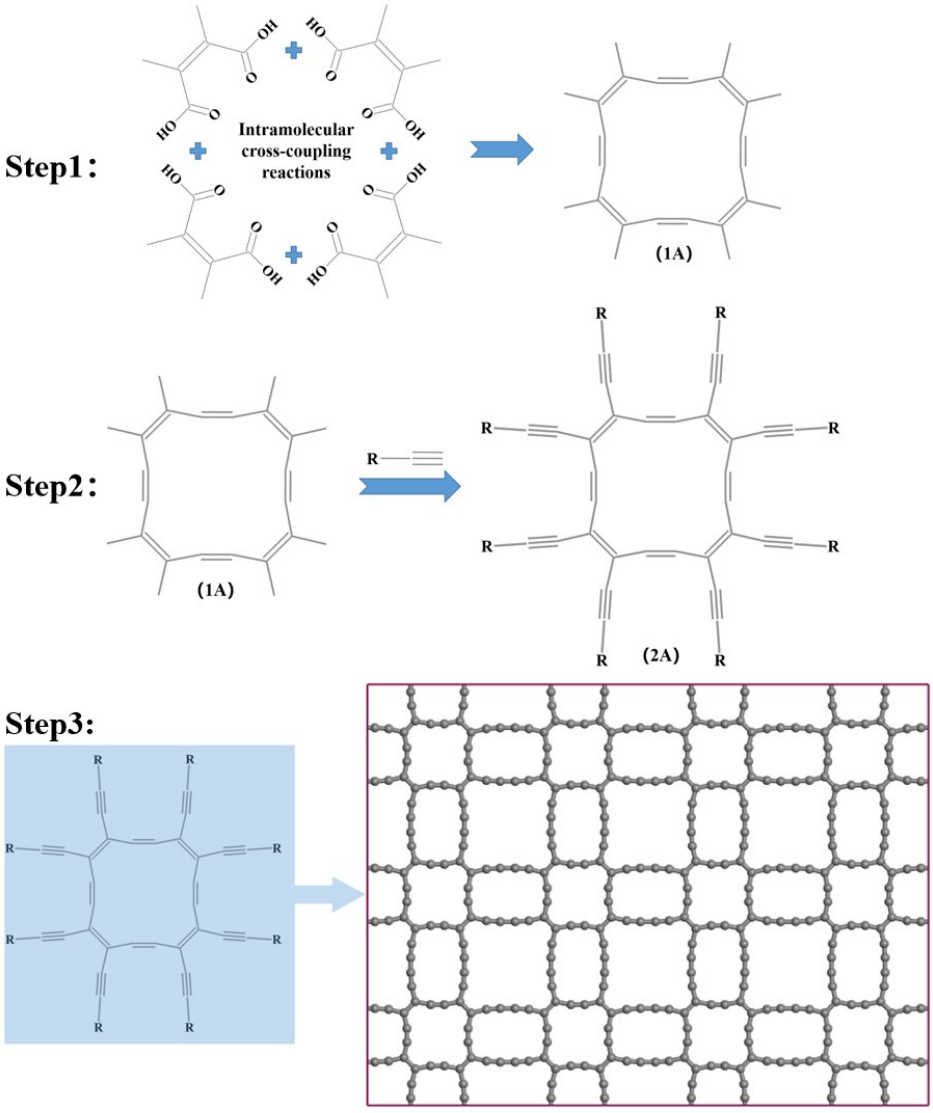

Figure S1. The possible synthetic route for 123-E8Y24-1.

II. The thermal stability of 123-E8Y24-1 with high temperature

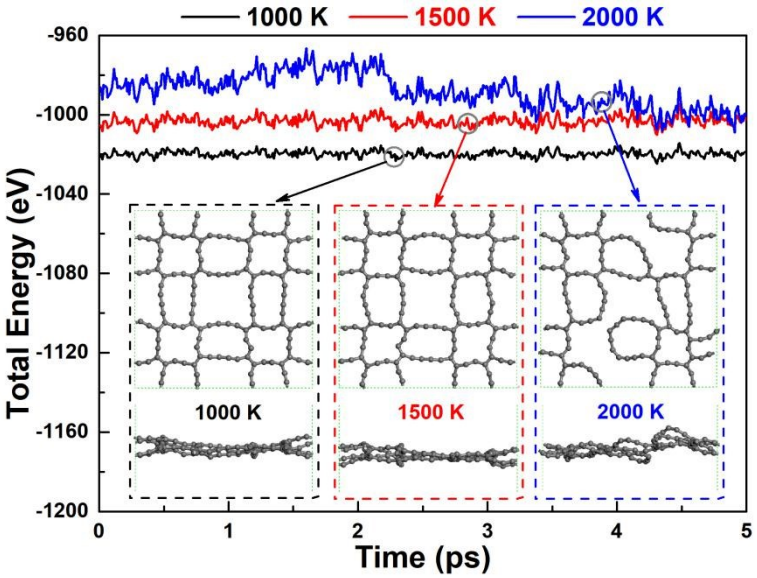

Figure S2. The fluctuations of average energies as function of simulation time for 123-E8Y24-1 with three typical temperature. The insets are the corresponding snapshots of atomic configuration for 123-E8Y24-1 with 2×2×1 supercell.

It is obviously that the geometric structure of 123-E8Y24-1 could be still maintained under 1500 K. As the temperature increases to 2000 K, however, both the fundamental structure and stable total energy of this new graphyne allotrope could not be preserved no longer. This result confirm that the 123-E8Y24-1 proposed in our work could withstand high temperature up to 1500 K.

III. The electronic band structure of 123-E8Y24-1 based on HSE06 hybrid function

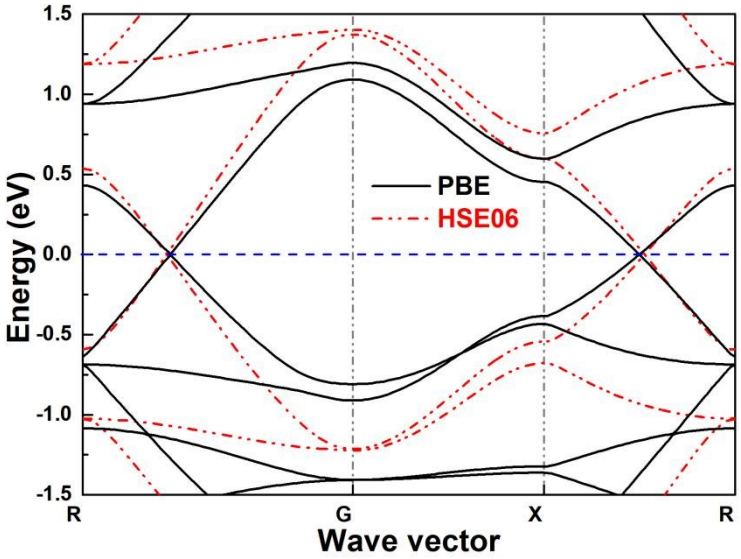

Figure S3. Electronic band structure of 123-E8Y24-1 along high-symmetry path by using PBE potential and HSE-06 hybrid functional potential.

Based on the HSE06 method, two bands still cross linearly at the Fermi level, which is similar to the result of PBE and further confirms the 123-E8Y24-1 presents a semimetal nature and possesses Dirac-nodal line states in the electronic band structure.

IV. The edge state of 123-E8Y24-1 nanoribbons

By means of tight-binding (TB) model, we calculate the electronic band structure of the 123-E8Y24-1 nanoribbon as well as projected edge band structures (yellow dots), and the results are depicted in Fig. S3. One can note clearly that there exist an obvious topological edge states.

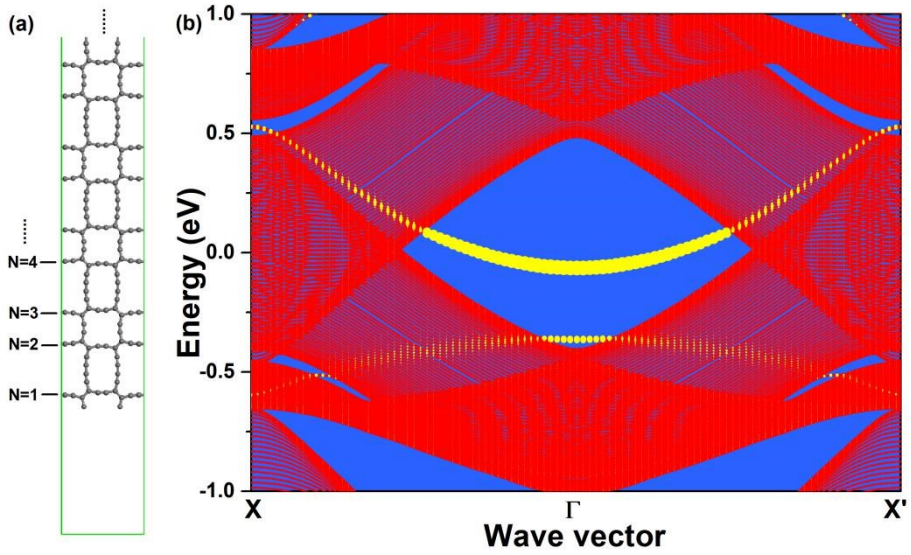

Figure S4. (a) Schematic representations and width definition of 123-E8Y24-1 nanoribbon. (b) Electronic band structure of 123-E8Y24-1 nanoribbon with width N=120 (bulk and edge structure are respeciviely represented by the red line and yellow dots).

V. The electronic structure of 123-E8Y24-1 with structural fluctuation

2D materials always display ripples with finite temperature, which will give rise to the broken of symmetry protection. Taken a simple rippled case as an example, we evaluate this effect on the electronic band structure of 123-E8Y24-1. One can find Fig. S5 that the rippled 123-E8Y24-1 opens a slight band gap about 0.85 meV. Such small band gap plays weak influence on the electronic properties of 123-E8Y24-1. That is to say, the main characters could be preserved well for the system with weak structural fluctuation (ripples).

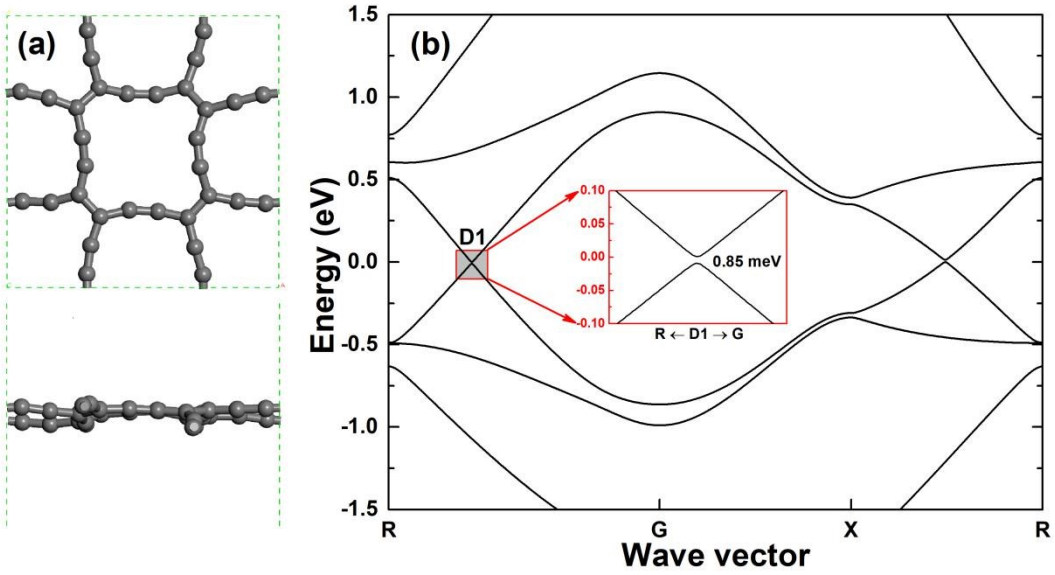

Figure. S5. (a) The atomic configuration of rippled 123-E8Y24-1 (obtained from the MD simulation with temperature 300 K). (b) The corresponding Electronic band structure along high-symmetry path by using PBE potential.The inset is the enlarged electronic band structure around the first Dirac-cone (D1).