Supporting Information of

Auxetic ographene: a new 2D Dirac nodal-ring semimetal carbon-base materials with high negative Poisson's ratio

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Section S1. The POSCAR Of Ographene

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ographene
1.0
        6.6259999275        0.0000000000        0.0000000000
        0.0000000000        6.6259999275        0.0000000000
        0.0000000000        0.0000000000       10.0000000000
     C
    18
Direct
      0.000000000         0.000000000         0.500000000
      0.500000000         0.500000000         0.500000000
      0.000000000         0.784169972         0.562789977
      0.000000000         0.215830028         0.562789977
      0.715830028         0.500000000         0.562789977
      0.284169972         0.500000000         0.562789977
      0.500000000         0.284169972         0.437210023
      0.500000000         0.715830028         0.437210023
      0.784169972         0.000000000         0.437210023
      0.215830028         0.000000000         0.437210023
      0.811779976         0.688220024         0.542779982
      0.188220024         0.311779976         0.542779982
      0.811779976         0.311779976         0.542779982
      0.188220024         0.688220024         0.542779982
      0.688220024         0.188220024         0.457220018
      0.311779976         0.811779976         0.457220018
      0.688220024         0.811779976         0.457220018
      0.311779976         0.188220024         0.457220018
```

Section S2. Synthesis of ographene

The possible synthesis route is given in Figure S5. According to the previous study[1], surface-assisted coupling method was used to product of atomically precise graphene nanoribbons with different topologies and widths. In addition, the on-surface synthesis method was also used to synthesize to large-area novel 2D carbon allotropes[2].

The topology structure of ographene can be well-defined by following the procedure in Figure S5.

Figure S1. (a) The total potential energy and (b-c) equilibrium structures of ographene at 300 and 1500 K during AIMD simulations.

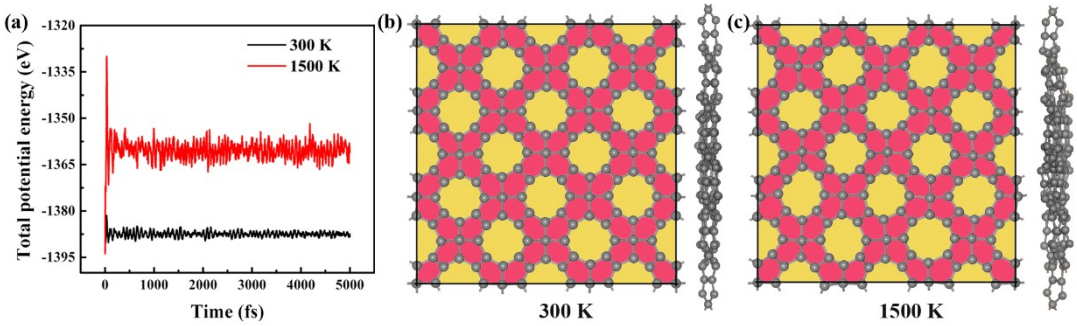


Figure S2. (a) The parameters of t_{ij} and (b) band structures of ographene calculated by the TB method and compared with PBE. Fermi level has been set to zero.

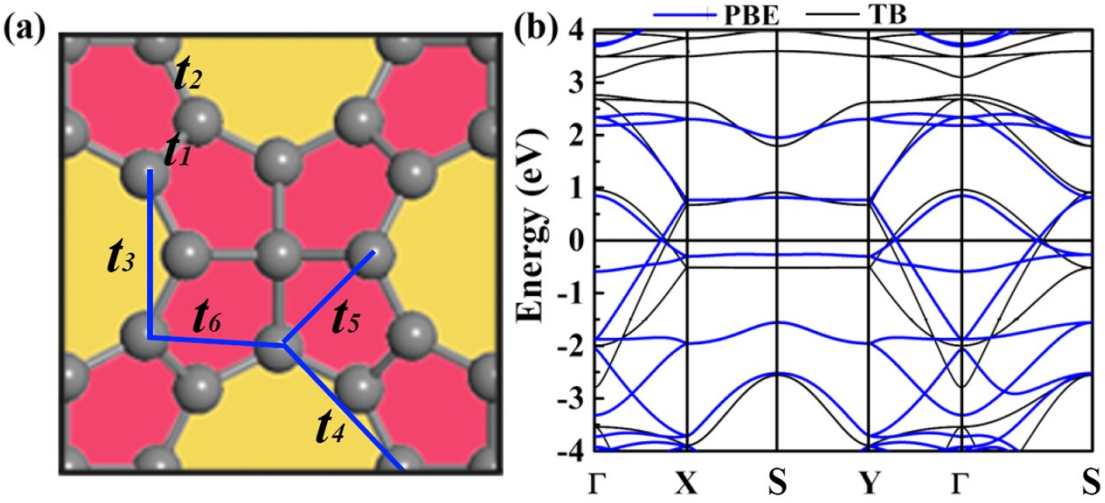


Figure S3. (a) Band structures of ographene calculated by the SOC method. The band structures are enlarged along the Γ–X and Γ–Z paths. Fermi level has been set to zero.

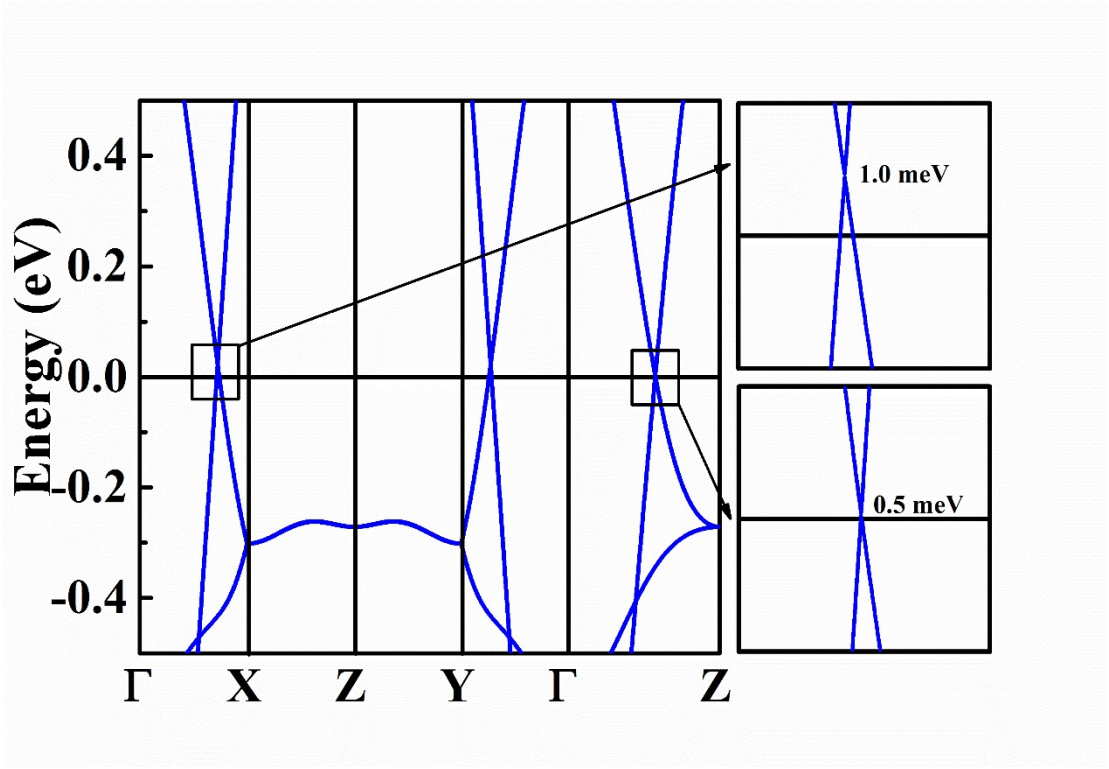


Figure S4. The phonon spectra of ographene under uniaxial, biaxial, shear, and biaxial-shear loading at the strain of 5%

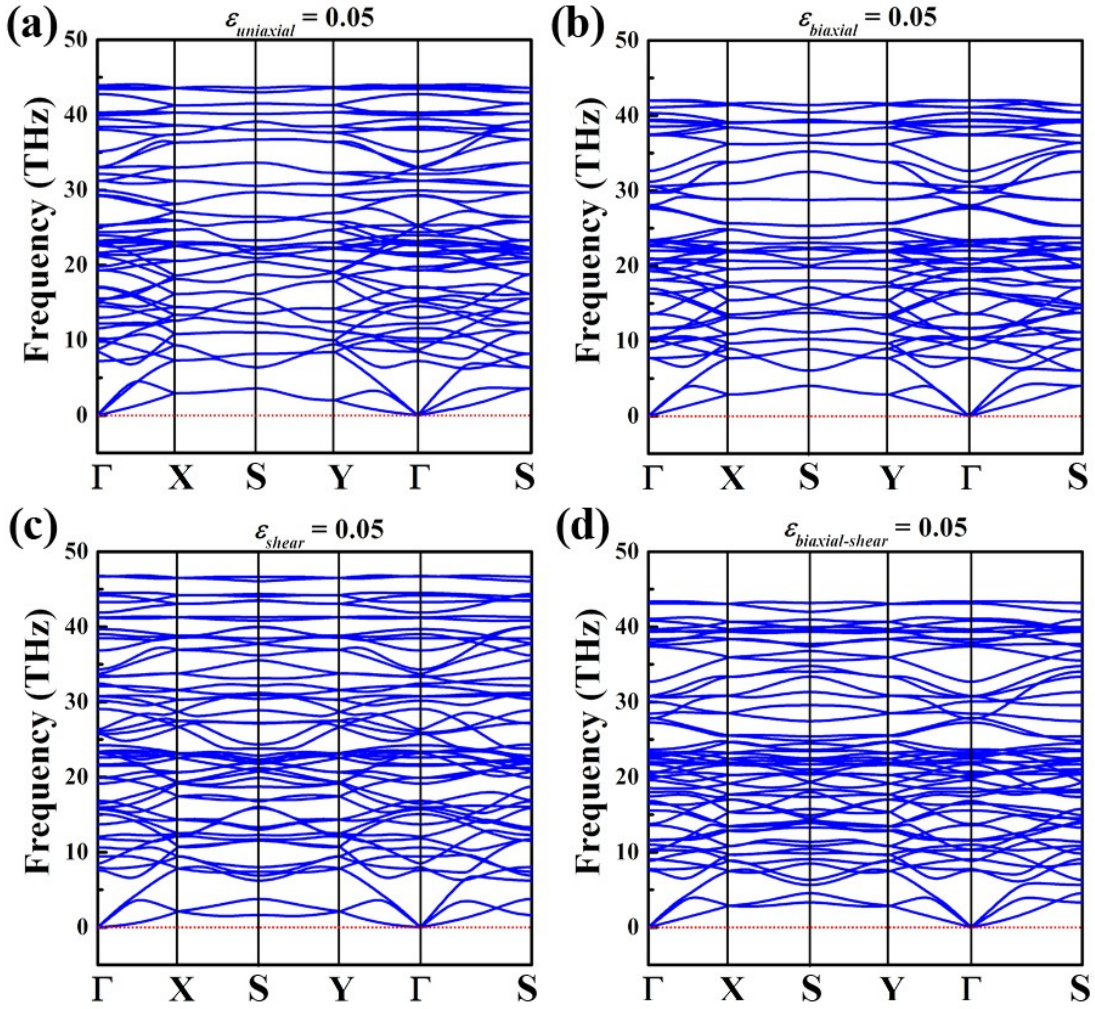
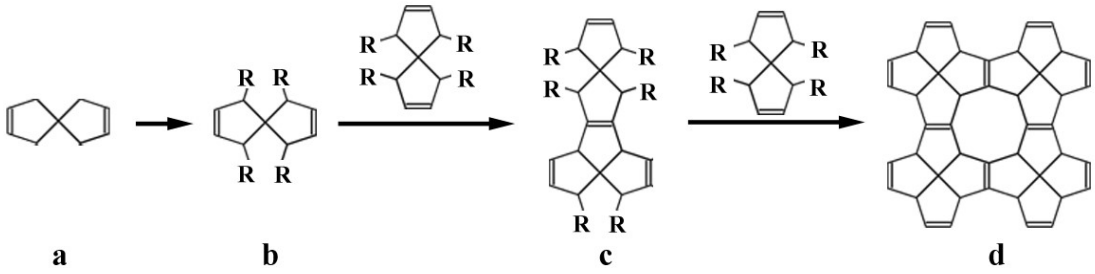


Figure S5. The possible synthesis route of ographene.



References

1. Cai, J.; Ruffieux, P.; Jaafar, R.; Bieri, M.; Braun, T.; Blankenburg, S.; Muoth, M.; Seitsonen, A. P.; Saleh, M.; Feng, X.; Müllen, K.; Fasel, R. Atomically precise bottom-up fabrication of graphene nanoribbons. *Nature* **2010,** *466* (7305), 470-473.

2. Fan, Q.; Martin-Jimenez, D.; Ebeling, D.; Krug, C. K.; Brechmann, L.; Kohlmeyer, C.; Hilt, G.; Hieringer, W.; Schirmeisen, A.; Gottfried, J. M. Nanoribbons with Nonalternant Topology from Fusion of Polyazulene: Carbon Allotropes beyond Graphene. *Journal of the American Chemical Society* **2019,** *141* (44), 17713-17720.