

Supporting information

A planar T-carbon structure with tunable electric and optical properties via chemical decorations on (111) plane: a first-principles investigation

Haifang Cai ^{a#}, Zhiwen Duan ^{b#}, Kun Cai ^{b*}, Douglas S. Galvao ^{c*}, and Qinghua Qin ^{d*}

^a School of Civil Engineering, Yan' an University, Yan' an 716000, China

^b School of Science, Harbin Institute of Technology, Shenzhen 518055, China

^c Applied Physics Department and Center for Computational Engineering & Sciences - CCES, State University of Campinas, Campinas, SP 13081-970, Brazil.

^d Institute of Advanced Interdisciplinary Technology, Shenzhen MSU-BIT University, Shenzhen 518172, China

*Corresponding authors' email addresses: kun.cai@hit.edu.cn (K.C.); galvao@ifi.unicamp.br (D.S.G.); Qinghua.qin@anu.edu.cn (Q.H.Q)

[#]These authors contributed equally to this work

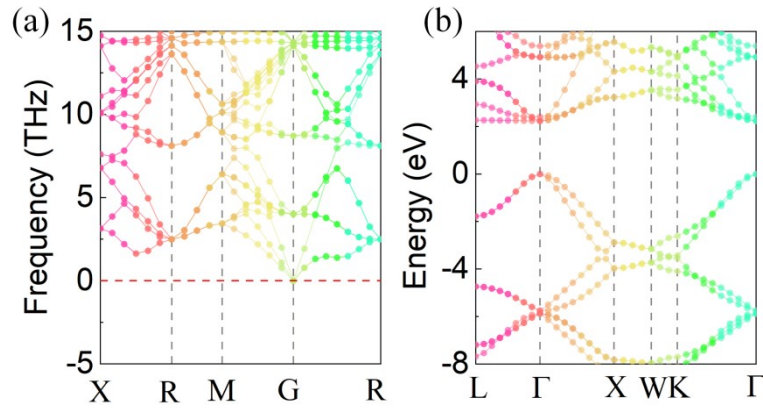


Fig. S1. The (a) phonon spectrum and (b) band structure of optimized bulk T-carbon.

Fig. S1 shows the (a) phonon spectrum and (b) band structure of optimized bulk T-carbon. The phonon spectrum of the bulk T-carbon has no imaginary frequencies along the entire Brillouin zone (S1 (a)). Its electronic band structure (S1 (b)) is consistent with the reports calculated using the VASP package. This agreement validates the rationality of our computational models and parameters, ensuring the reliability of subsequent surface-decorated system simulations.

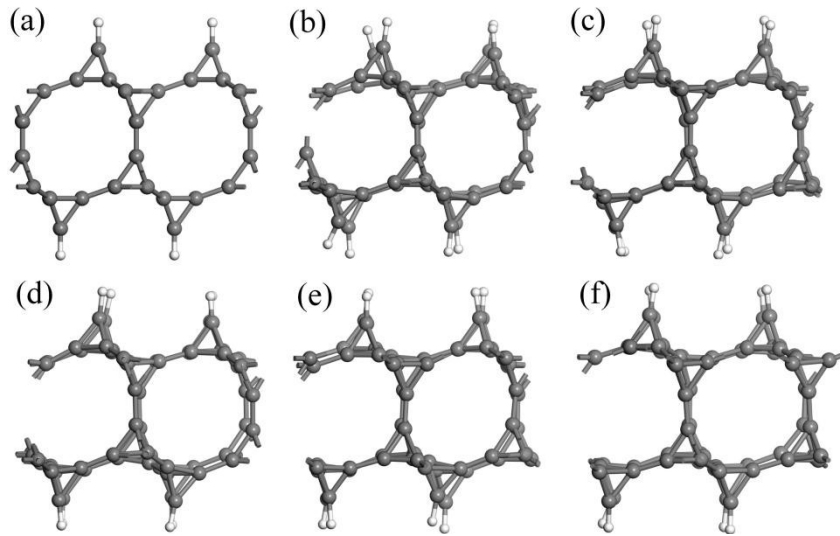


Fig. S2. Snapshots of -H decorated 2-(111) planar T-carbon under 300 K at (a) 0 ps, (b) 1 ps, (c) 2 ps, (d) 3 ps, (e) 4 ps and (f) 5 ps. Here, the lattice line is concealed.

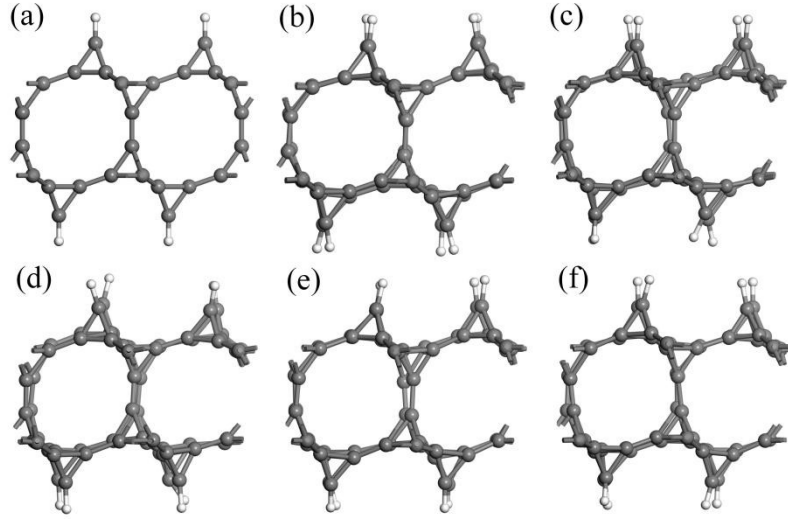


Fig. S3. Snapshots of -H decorated 2-(111) planar T-carbon under 500 K at (a) 0 ps, (b) 1 ps, (c) 2 ps, (d) 3 ps, (e) 4 ps and (f) 5 ps. Here, the lattice line is concealed.

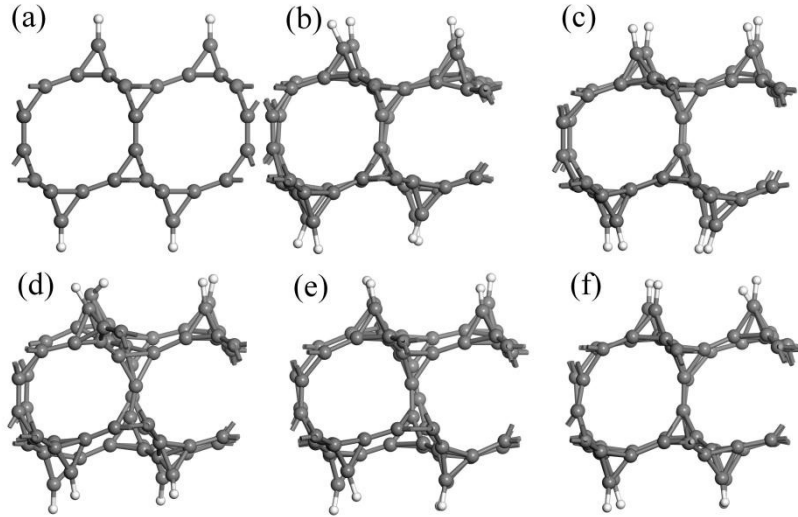


Fig. S4. Snapshots of -H decorated 2-(111) planar T-carbon under 700 K at (a) 0 ps, (b) 1 ps, (c) 2 ps, (d) 3 ps, (e) 4 ps and (f) 5 ps. Here, the lattice line is concealed.

Fig. S2, S3 and S4 are snapshots of -H decorated 2-(111) planar T-carbon under 700 K at (a) 0 ps, (b) 1 ps, (c) 2 ps, (d) 3 ps, (e) 4 ps and (f) 5 ps, respectively. These snapshots reveal that no significant structural distortion is observed in the -H decorated 2-(111) planar T-carbon under thermal conditions ranging from room temperature up to elevated temperatures of 500 K and 700 K, demonstrating its thermodynamic stability. This further confirms that surface decoration effectively enhances the structural stability of the material.