

Electronic Supplementary Information

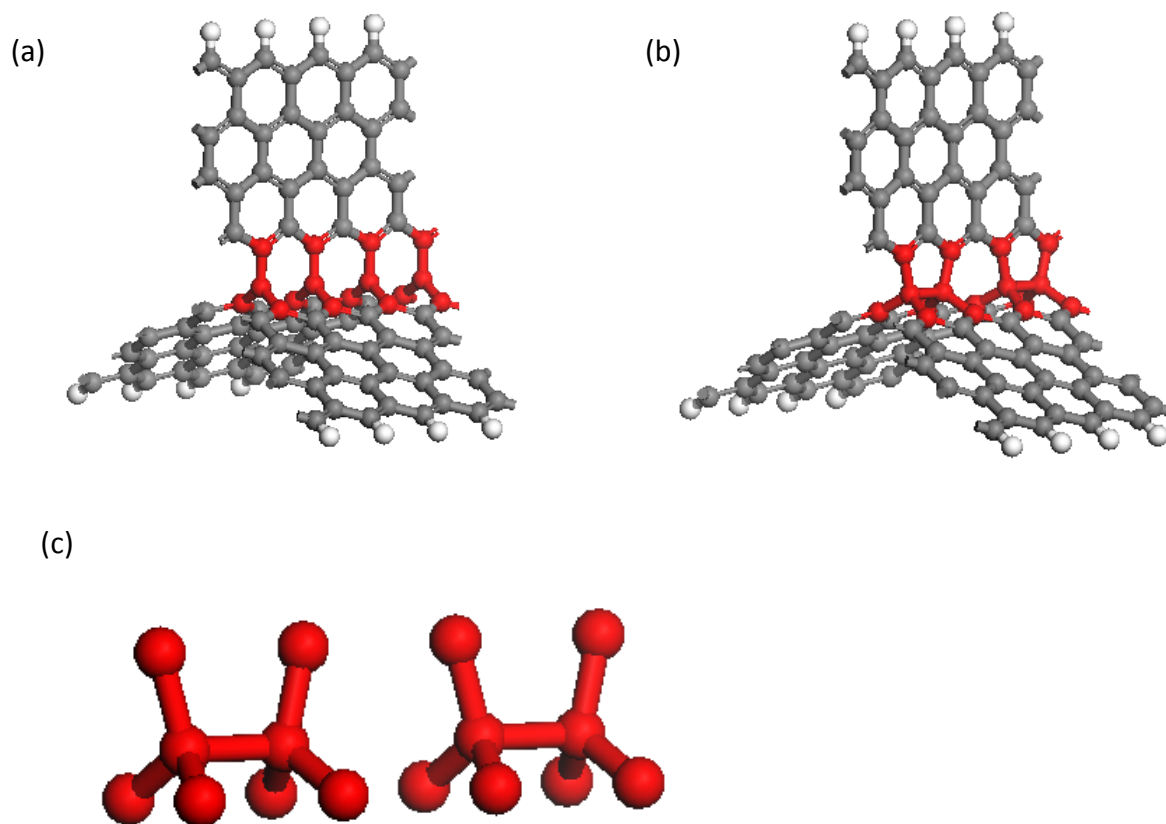
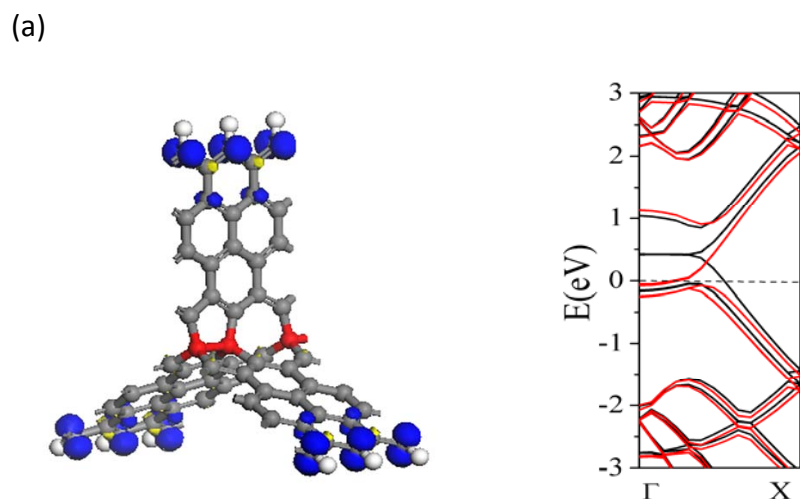


Figure S1 Geometric structures of cc-TWG nanoribbon (a) prior to and (b) after the formation of carbon-carbon dimers along the center carbon chain. The zig-zag edges of the TWG nanoribbon are fully passivated by hydrogen atoms. (c) is an enlarged illustration of the joint section. Carbon atoms in the center and their connected neighbor carbon atoms are highlighted in red.



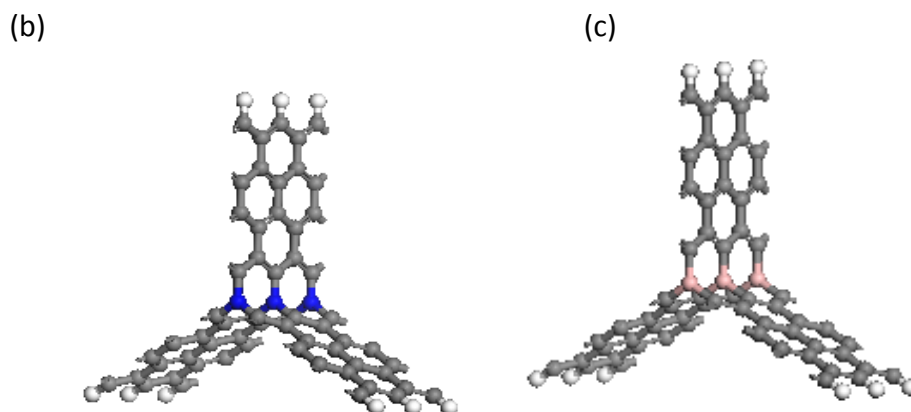


Figure S2 (a) The spin-density distribution and band structure of the cc-TWG nanoribbon. (b) and (c) show structures of nitrogen-centered and boron-centered TWG nanoribbon, respectively. Grey, white, blue, pink balls denote carbon, hydrogen, nitrogen and boron atoms. Carbon atoms in the center are highlighted in red. In (a), blue and yellow represent spin-up and spin-down spin state, respectively, and the range of iso-value spin density is $[-0.03, 0.03]$. Black lines represent the spin-up channel and red lines represent the spin-down channel, the black dashed line denotes the Fermi level.

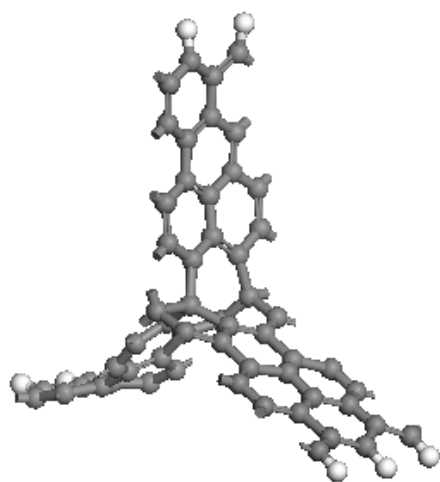


Figure S3. A snapshot of the equilibrium structure of cc-TWG nanoribbons at 1000 K and at the end of 5 ps quantum (Born-Oppenheimer) molecular dynamics simulation. Specifically, the constant-temperature and constant-volume (*NVT*) ensemble is chosen and the Nosé-Hoover chain method [Martyna, G. J.; Klein, M. L.; Tuckerman, M. E. *J. Chem. Phys.* 1992, **97**, 2635] is used for temperature control (the temperature is fixed at 1000 K). The Nosé Q ratio is set 2.0 and the Nosé chain length is 2.

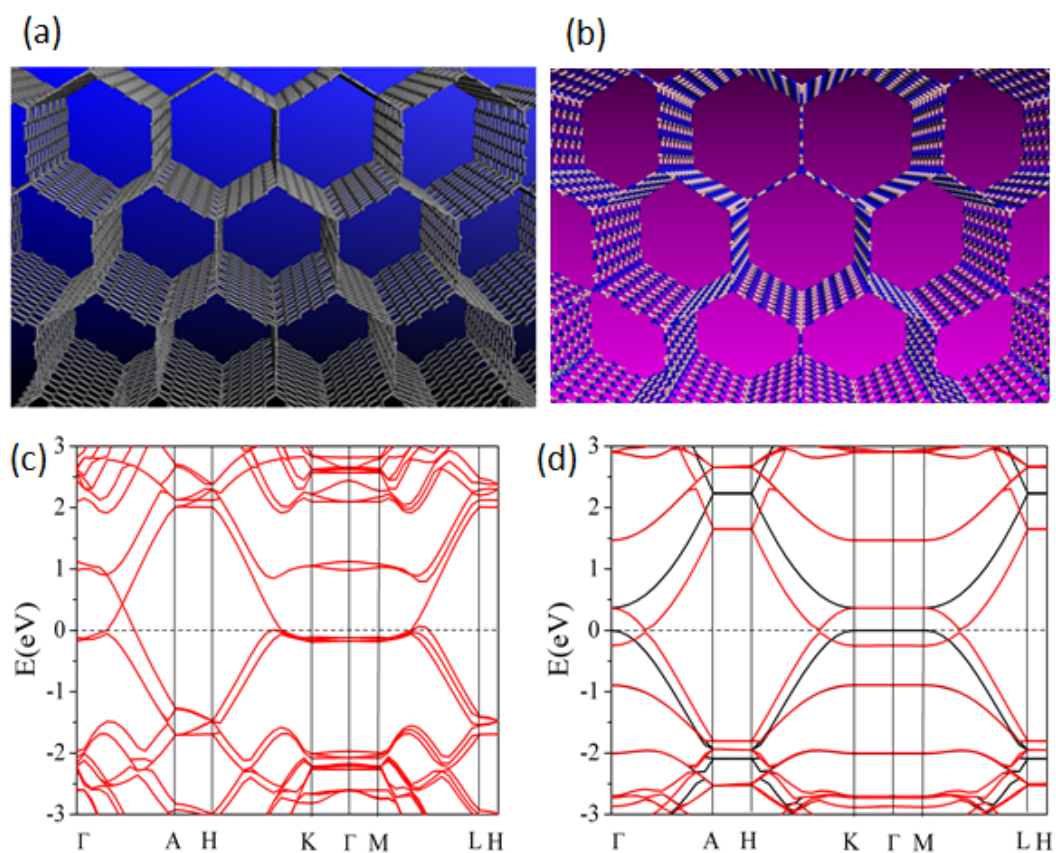


Figure S4 Geometry and electronic band structures of the honeycomb (a) (c) carbon and (b) (d) BN foam. $\Gamma(0.0, 0.0, 0.0)$, A(0.0, 0.0, 0.5), H(-0.333, 0.667, 0.5), K(-0.333, 0.667, 0.0), M(0.0, 0.5, 0.0), and L(0, 0.5, 0.5) refer to special symmetry points in the first Brillouin zone.

Table S1. Calculated Young's modulus and bulk modulus of the carbon and BN foams.

	honeycomb carbon	honeycomb BN	triangular carbon	triangular BN
E_x (GPa)	30	35	288	232
E_z (GPa)	339	255	641	502
B_0 (GPa)	72	64	202	145