Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for Asymmetric passivation of edges: a route to make magnetic graphene nanoribbon

Wen-cai Yi,[ab] Wei Liu,[cd] Lei Zhao,[b] Rashed Islam,[b] Mao-sheng Miao*[bc] and Jing-yao Liu*[a]

[a] *Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, People's Republic of China. E-mail: ljy121@jlu.edu.cn;*

[b] *Department of Chemistry & Biochemistry, California State University, Northridge, CA, 91330, USA. E-mail: mmiao@csun.edu*

[c] *Beijing Computational Science Research Center, Beijing, 100094, P. R. China*

[d] *Department of Physics and Astronomy, University of California, Irvine, CA, 92697, USA*

Table S1: The value of band gap of the studied ZGNRs (at PBE level)

Name	8-ZGNR	8-ZGNR-1/8	8-ZGNR-4/8	8-ZGNR-8/8
Band gap (eV)	0.67	0.26	0.06	0.09

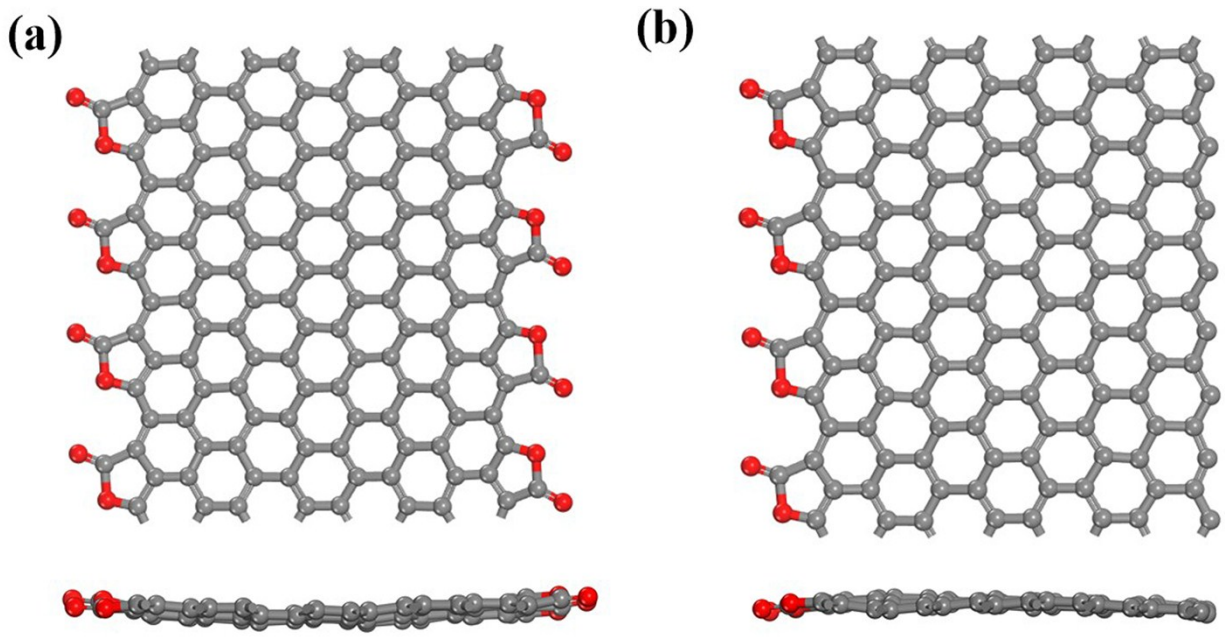

Fig. S1: The top and side view of the final configurations for each molecular dynamics simulation at 400K of (a) 8-ZGNR-8/8 and (b) 8-ZGNR-4/8, respectively.

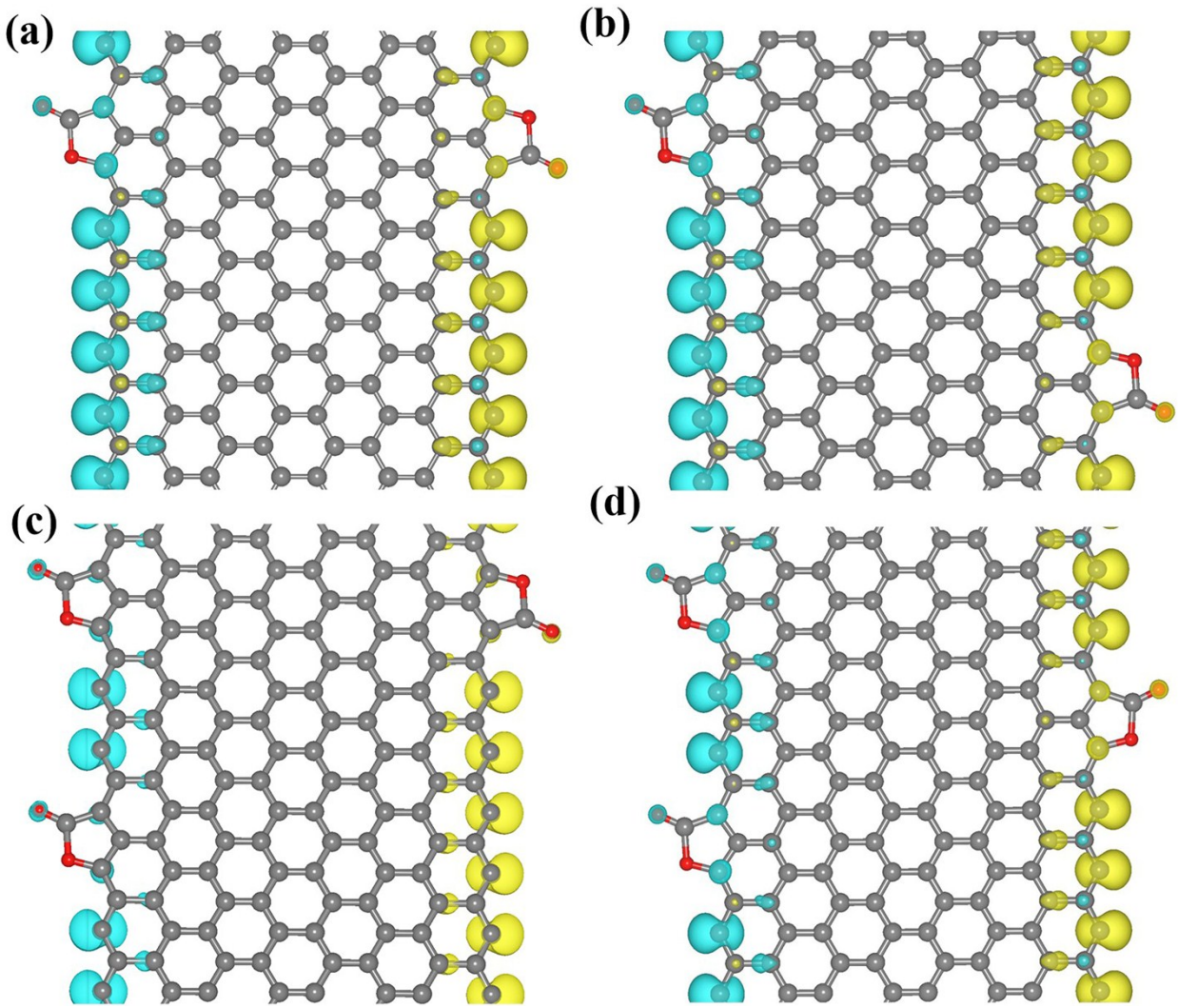

Fig. S2: The spin-polarized electron density of (a) two CO_2 molecules adsorbed on two edges of 8-ZGNR, AFM, m= 0.00μ_B; (b) two CO_2 molecules adsorbed on two different position of edges of 8-ZGNR, AFM, m= 0.00μ_B; (c) three CO_2 molecules adsorbed on two edges of 8-ZGNR, AFM, m= 2.00μ_B; (d) three CO_2 molecules adsorbed on three different position of edges 8-ZGNR, AFM, m= 2.00μ_B; bule was spin up and yellow was spin down. The isosurface value is set to 1.00 $\times 10^{-2}$ $Å^{-3}$.

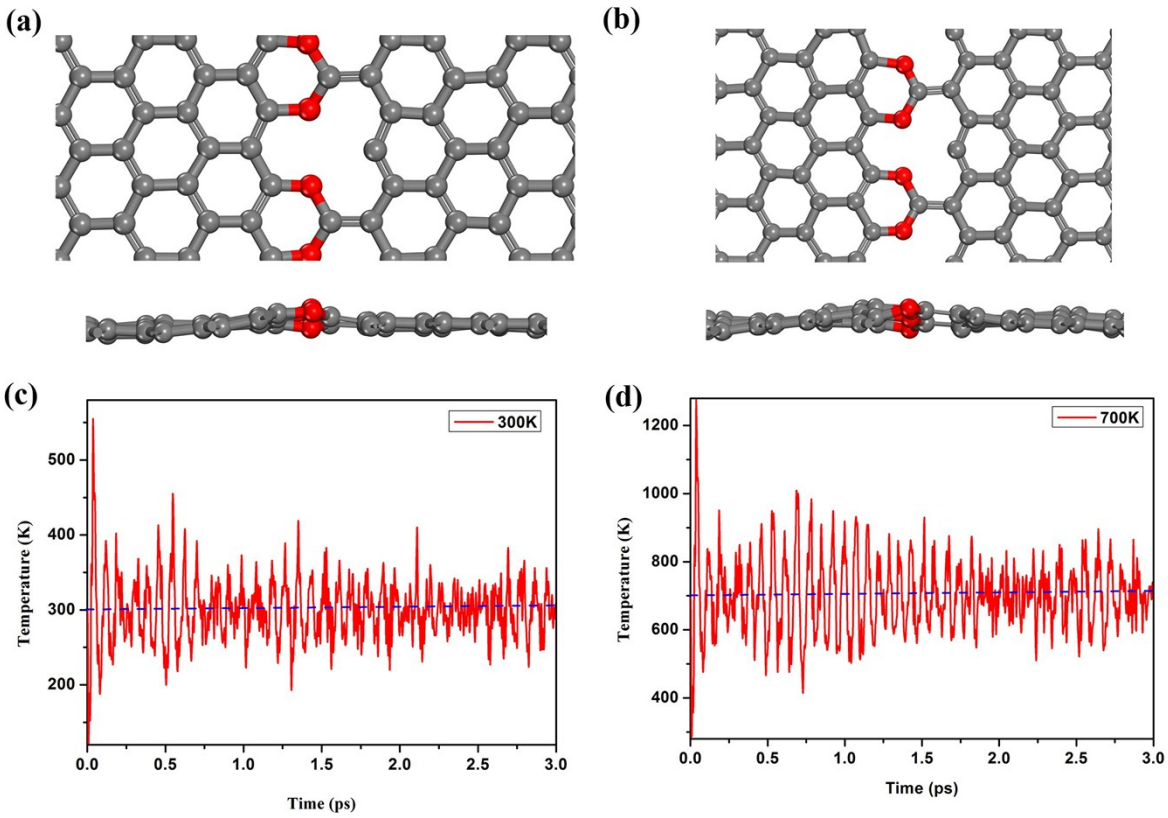

Fig. S3: Snapshots of the final configurations for each molecular dynamics simulation under (a) 300 and (b) 700 K (top and side views); The fluctuations of temperature as a function of the molecular dynamic simulation step at (c) 300K and (d) 700 K, respectively.