Carbon Nanoscroll from C$_4$H/C$_4$F-type Graphene Superlattice: MD and MM Simulation Insights

Zilong Liu,$^{ab}$ Qingzhong Xue,*$^{abc}$ Yehan Tao,$^b$ Xiaofang Li,$^b$ Tiantian Wu,$^b$

Yakang Jin$^b$ and Zhongyang Zhang$^b$

$^a$ State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Qingdao 266580, Shandong, P. R. China

$^b$ College of Science, China University of Petroleum, Qingdao 266580, Shandong, P. R. China

$^c$ Shengli-highland Limited Company, Dongying 257062, Shandong, P. R. China
**Fig.S1** The decrease in energy as a function of simulation time. (a) non-bonding energy and van der Waals (vdW) energy in C₄H scrolls of Fig.2a. (b) non-bonding energy and electrostatic energy in C₄F scrolls of Fig.2b.
Fig. S2 Functionalized directions: X-direction (a), Y-direction (b), and Diagonal direction (c) in C₄H/C₄F-type graphene superlattices. Grey, white, and blue balls represent C, H, and F atoms, respectively.
Fig.S3 Snapshots of CNS structures formed by various edge length (68.83, 144.73, 218.63 Å) of equilateral triangle of $C_4H$ (a1-c1) and $C_4F$ (a2-c2).