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

Simulation Insights

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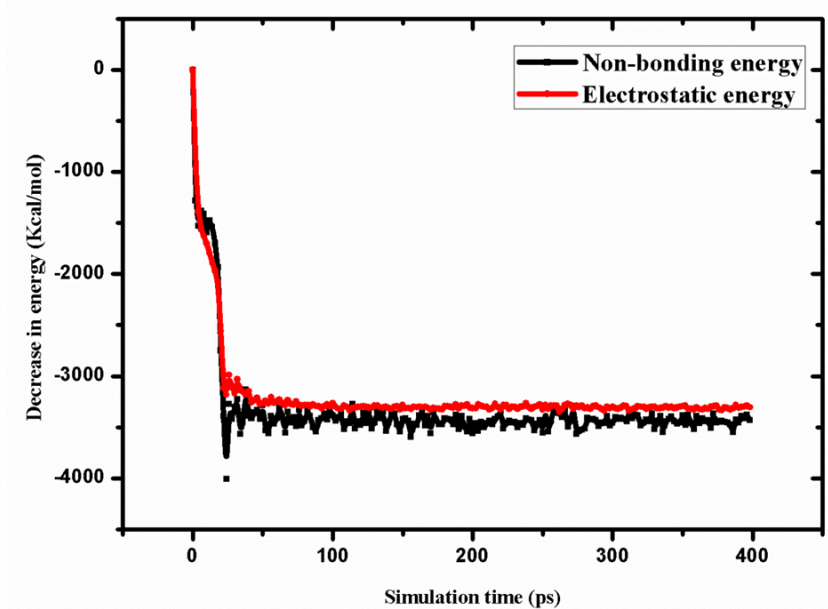
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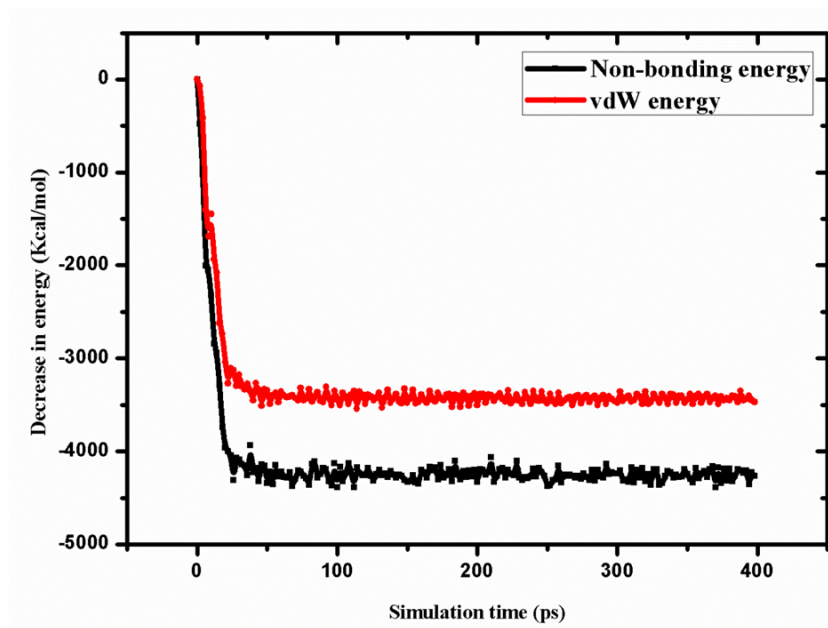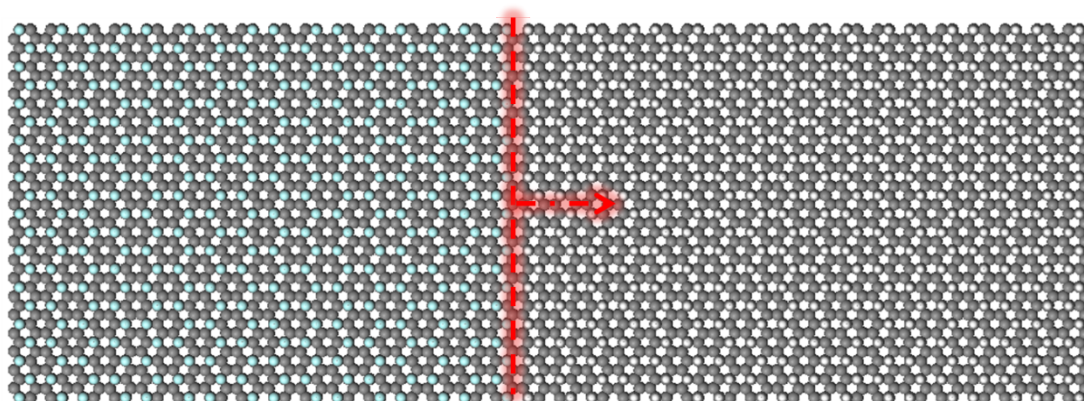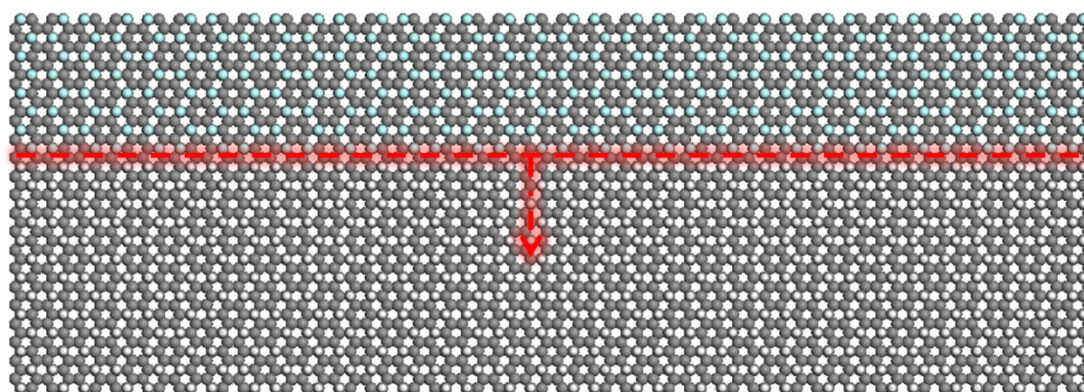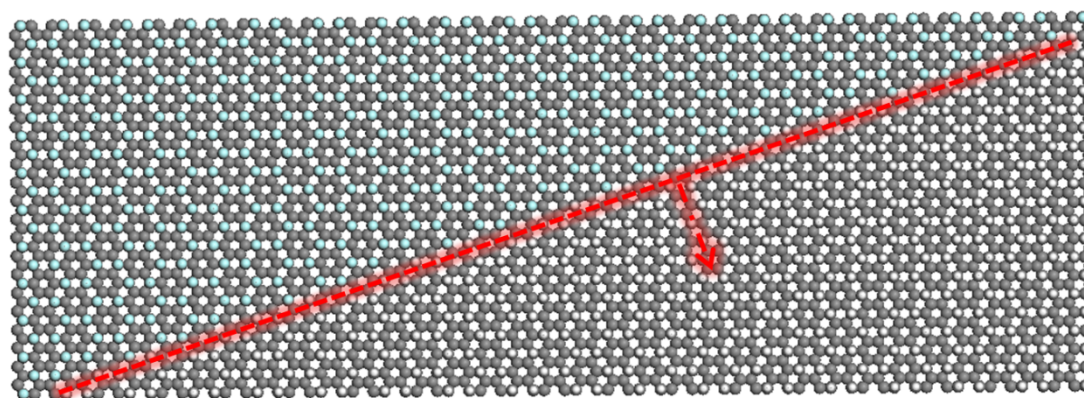
Fig.S1 The decrease in energy as a function of simulation time. (a) non-bonding energy and van der Waals (vdW) energy in C_4H scrolls of Fig.2a. (b) non-bonding energy and electrostatic energy in C_4F scrolls of Fig.2b.

(a)

(b)

(c)

Fig.S2 Functionalized directions: X-direction (a), Y-direction (b), and Diagonal direction (c) in C_4H/C_4F-type graphene superlattices. Grey, white, and blue balls represent C, H, and F atoms, respectively.
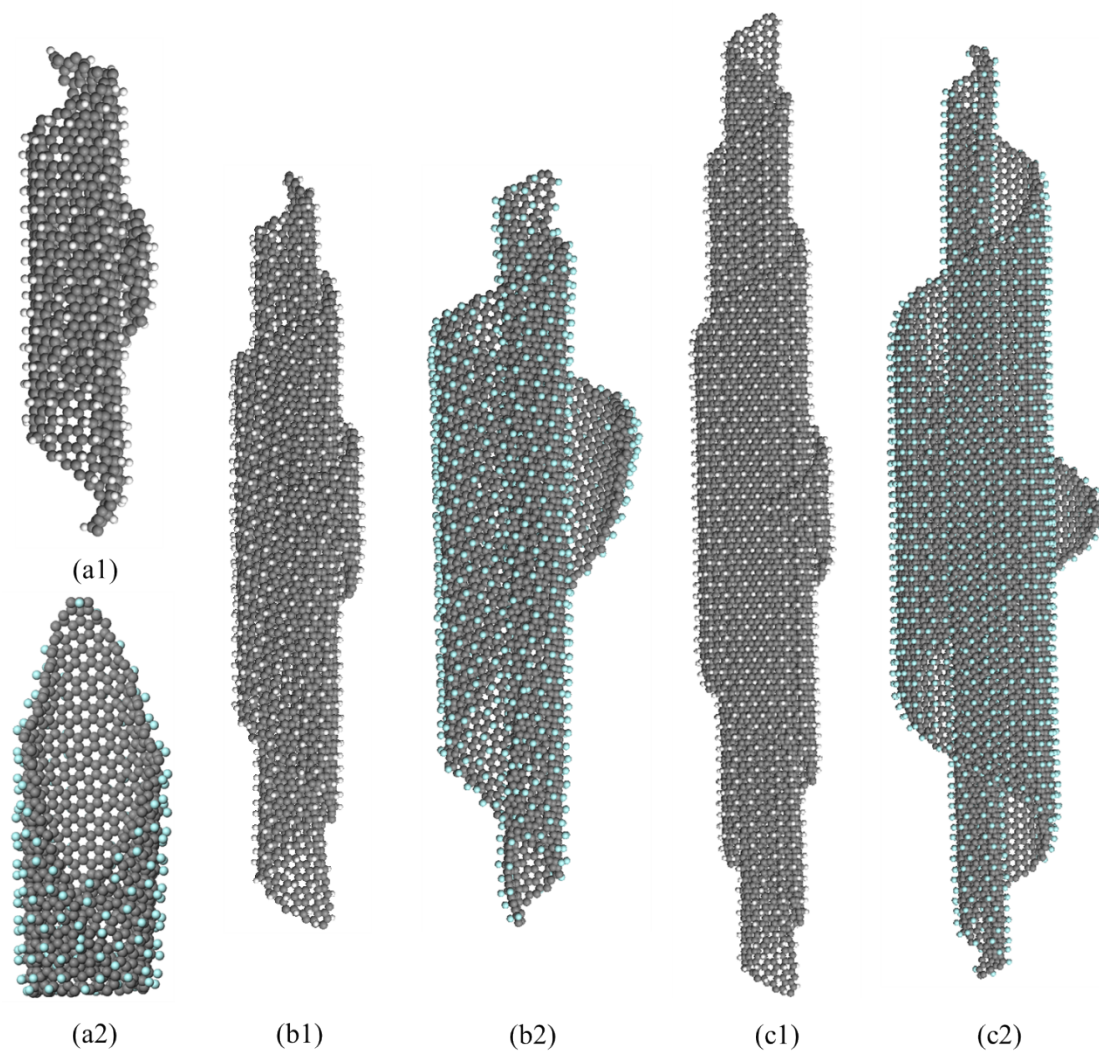
(a1)

(a2)   (b1)   (b2)   (c1)   (c2)

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).