

Supplementary Information for

Transformation of starphenes into amorphous graphene nanoribbons with attached carbon chains under electron irradiation

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Simulated structure evolution of the $C_{88}H_{46}$ starphene in vacuum under 45 keV electron irradiation in HRTEM

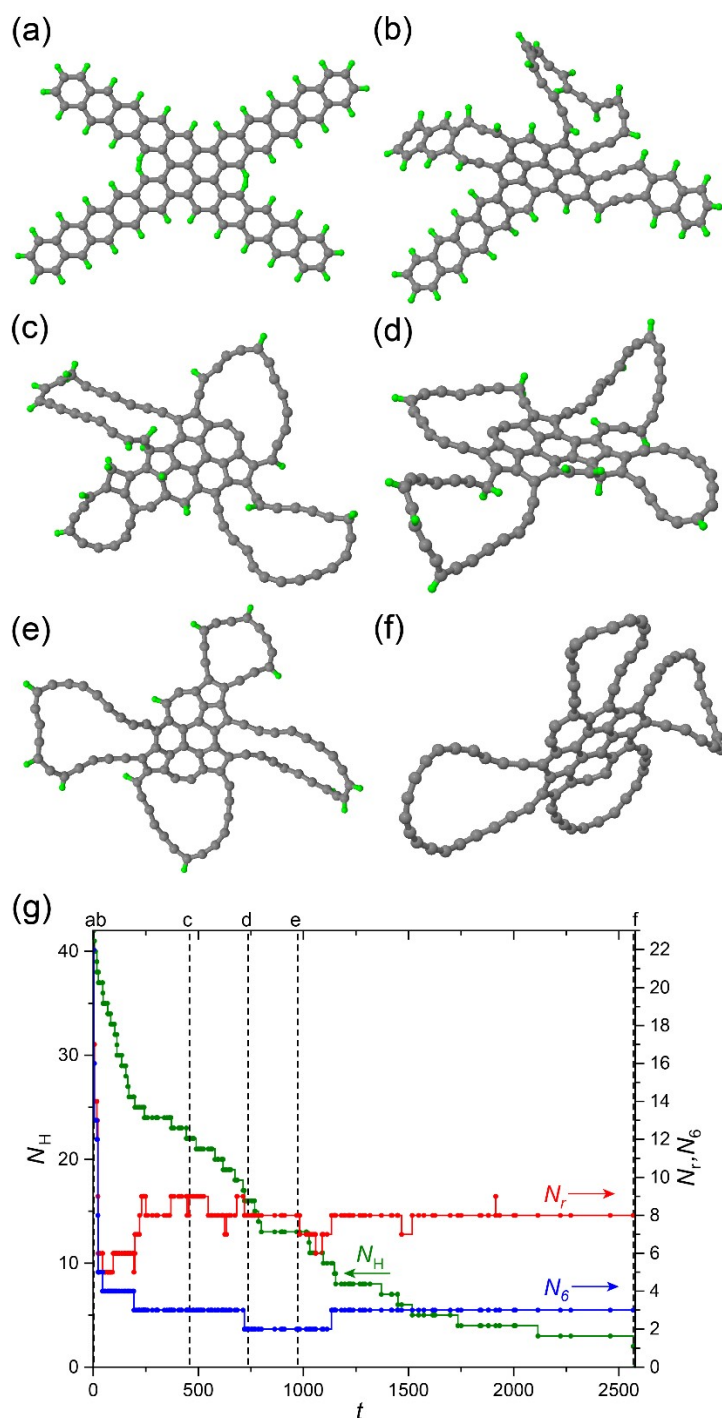


Figure S1. (a)–(f) Simulated structure evolution of the $C_{88}H_{46}$ starphene in vacuum under 45 keV electron irradiation in HRTEM: (a) 0 s, (b) 2.36 s, (c) 458.1 s, (d) 736.7 s, (e) 972.6 s and (f) 2568.2 s. The direction of the electron beam is out of the page. Carbon and hydrogen atoms are colored grey and green, respectively. (g) Calculated number of hydrogen atoms remaining attached to in the molecule, N_H (green line), , total number of 5-, 6-, 7-, and 8-rings, N_r (red line, right axis), and and number of hexagons in the molecule structure, N_6 (red line, right axis), and and number of hexagons in the molecule structure, N_6 (blue line), as functions of time t in the same simulation run. The moments of time corresponding to structures (a)–(f) are shown using vertical dashed lines.

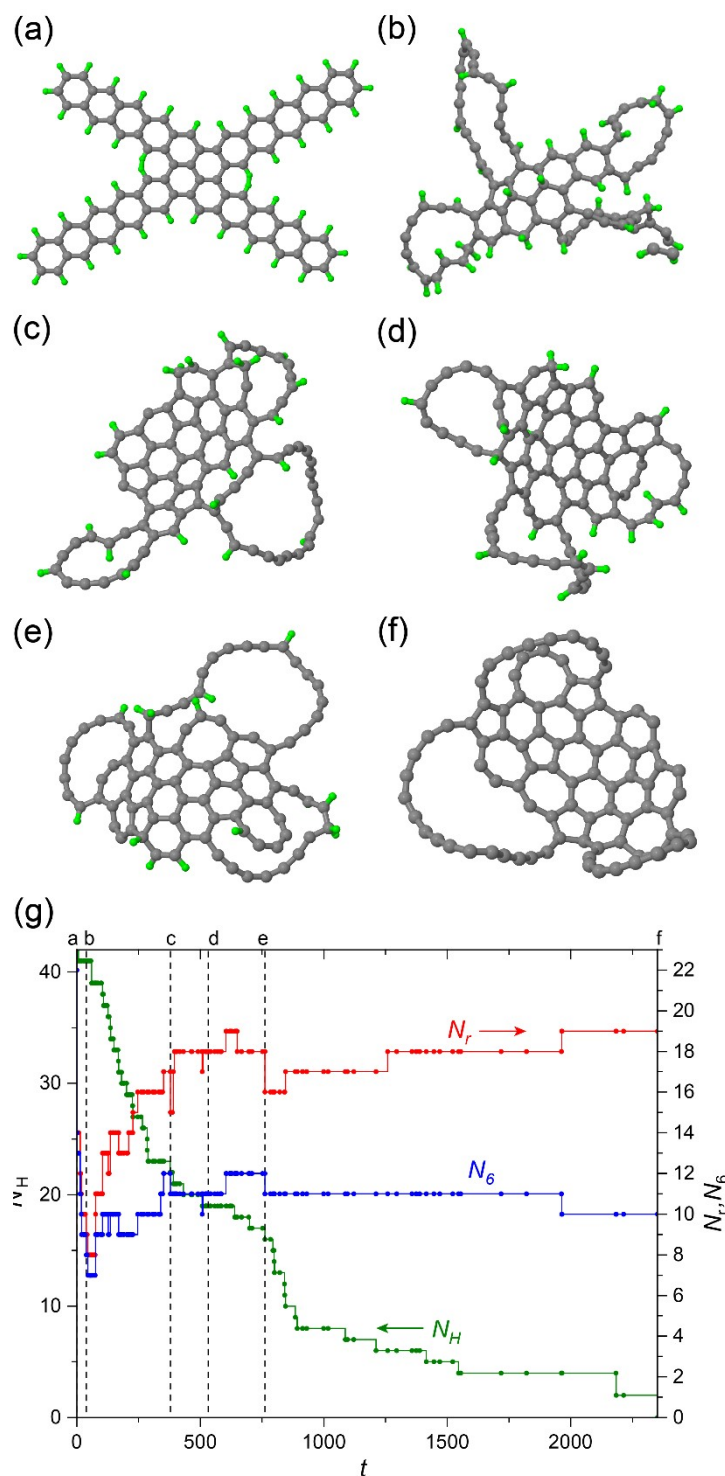
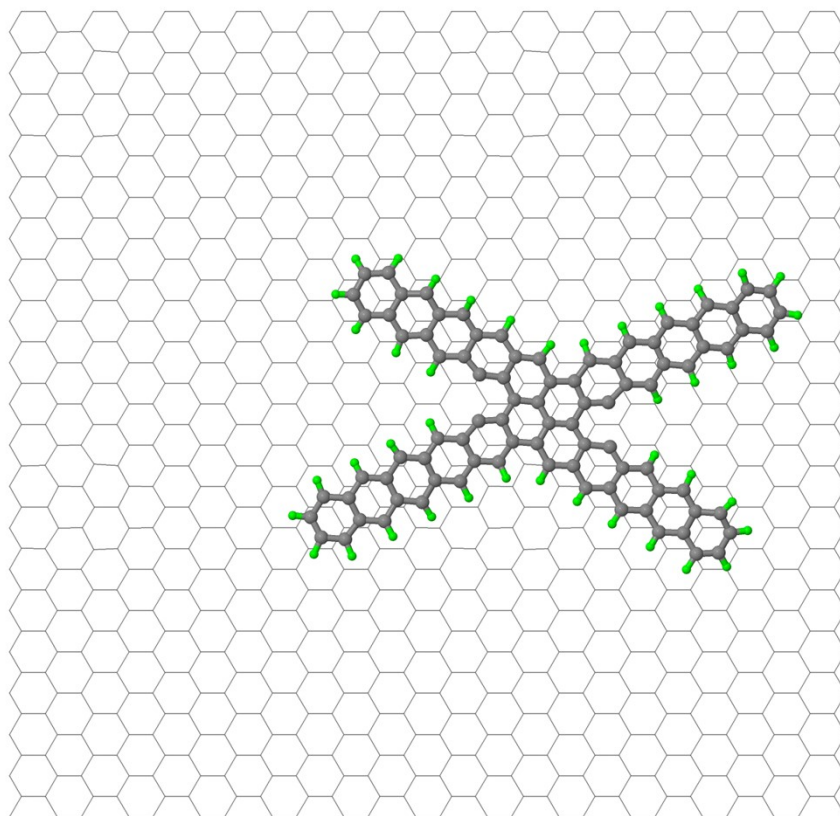


Figure S2. (a)–(f) Simulated structure evolution of the $C_{88}H_{46}$ starphene in vacuum under 45 keV electron irradiation in HRTEM: (a) 0 s, (b) 38.1 s, (c) 378.9 s, (d) 533.7 s, (e) 762.0 s and (f) 2351.4. s. The direction of the electron beam is out of the page. Carbon and hydrogen atoms are colored grey and green, respectively. (g) Calculated number of hydrogen atoms remaining attached to in the molecule, N_H (green line), , total number of 5-, 6-, 7-, and 8-rings, N_r (red line, right axis), and and number of hexagons in the molecule structure, N_6 (blue line), as functions of time t in the same simulation run. The moments of time corresponding to structures (a)–(f) are shown using vertical dashed lines.

Description of the video files attached

Video files “vid_cplm_graphene_45kev.avi” and “vid_agnr_graphene_45kev.avi” show examples of the structure evolution observed in the MD simulations during the formation of carbon propeller-like molecule and amorphous graphene nanoribbon with attached short carbon chains, respectively, from the $C_{88}H_{46}$ starphene on the graphene surface in HRTEM under electron irradiation with the electron kinetic energy of 45 keV. In this videos, all carbon and hydrogen atoms are colored in grey and green, respectively. The total time in HRTEM (converted from the MD simulation time) as well as the total numbers of carbon and hydrogen atoms NC and NH are also given at the bottom of the frame.

MD Simulation by CompuTEM (45 keV)



TIME 0.0 s; NC = 1048; NH =42

Jmol