Electronic supplementary information for

Transformation of a graphene nanoribbon into a hybrid 1D nanoobject with alternating double chains and polycyclic regions

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Distributions of successful electron impacts over the energies transferred to hydrogen and carbon atoms

The minimal transferred energies T_{min} used for hydrogen and carbon atoms are 1 and 5 eV, respectively. In 10 calculations with 80 keV energy for the chosen GNR structure, there are 2079 successful electron impacts producing structural changes. 675 (32%) out of these impacts are impacts on carbon atoms, 1404 are on hydrogen atoms (1362 (97%) resulting in knock-out of a hydrogen atom). The distributions of successful electron impacts over the energies transferred to hydrogen and carbon atoms show that most of the successful impacts occur at the energies that are significantly greater than the chosen values of T_{min} (see Figure S1). Thus, almost all successful electron impacts are taken into account with such a choice of T_{min}.

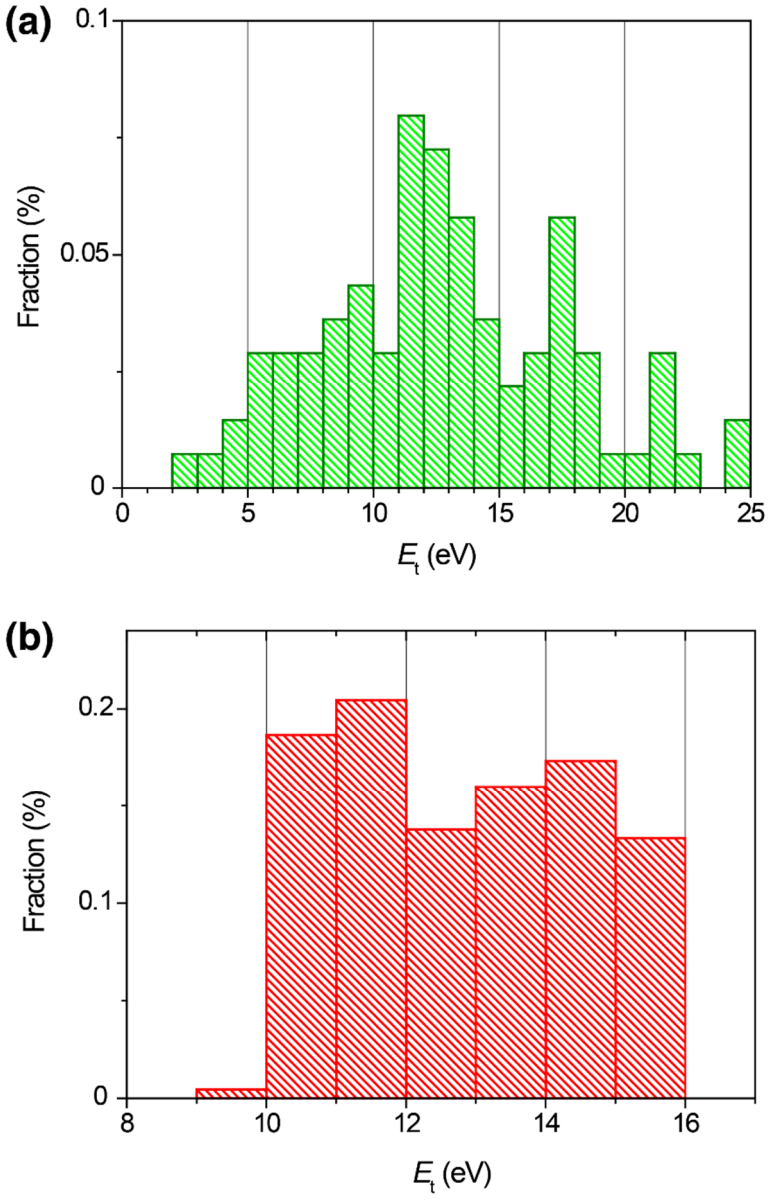


Figure S1. Calculated distributions of successful electron impacts over the energies transferred to hydrogen (a) and carbon (b) atoms. Each single bar shows the fraction of successful electron impacts (in %) corresponding to the given transferred energy E_t (in eV) within the interval of 1 eV. The minimal transferred energies T_{min} used for hydrogen and carbon atoms are 1 eV and 5 eV, respectively.

DFT studies of the 1D nanoobject with D1 polycyclic regions

Bond length alternation in carbon chains

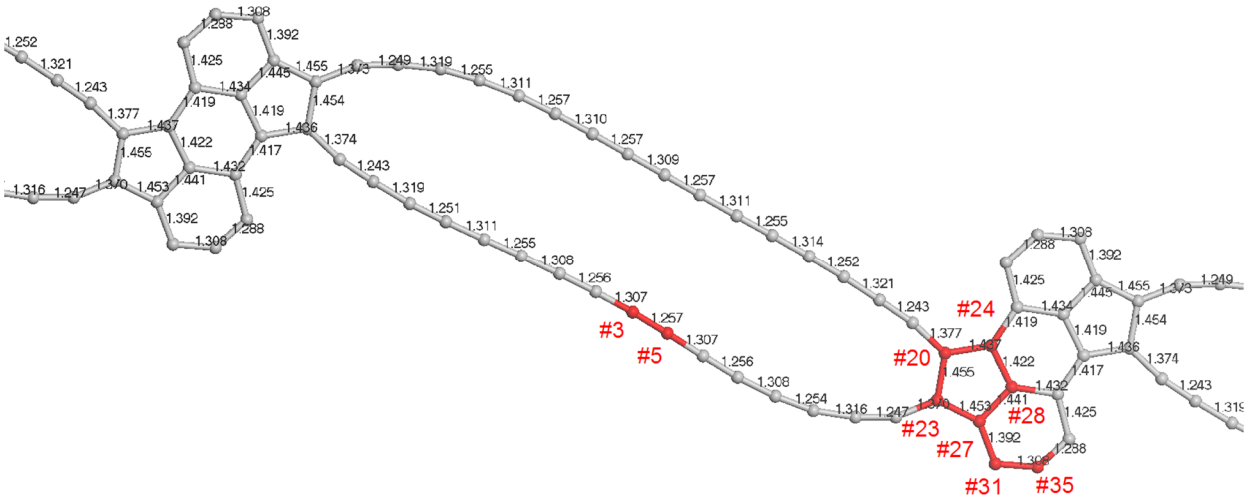


Figure S2. Geometrically optimized structure of the 1D nanoobject with D1 polycyclic regions obtained by the DFT calculations. The bond lengths (in Å) are indicated in grey. The atoms for which the partial densities of states are computed are shown in red.

The bond length alternation δ in carbon chains of the 1D nanoobject is computed according to papers [1,2] as

$$\delta = \frac{1}{2}\left|\frac{1}{n_e}\sum_{j=1}^{n_e}\left(d_{2j-1}+d_{n-(2j-1)}\right)-\frac{1}{n_0}\sum_{j=1}^{n_0}\left(d_{2j}+d_{n-2j}\right)\right|, \qquad \text{(S1)}$$

where $d_i = \left|\vec{r}_i - \vec{r}_{i+1}\right|$, n is the number of atoms in the chain, $n_e = (n+2)/4$, and $n_0 = n/4$ (integer part). The terminal bonds here are excluded.

In the 1D nanoobject under consideration, the chains are composed of 16 atoms each. Therefore, $n_e = n_0 = 4$. From the bond lengths shown in Figure S2, we get $\delta = 6.0$ pm and 5.8 pm for the upper and lower chains in this figure, respectively.

Partial densities of states

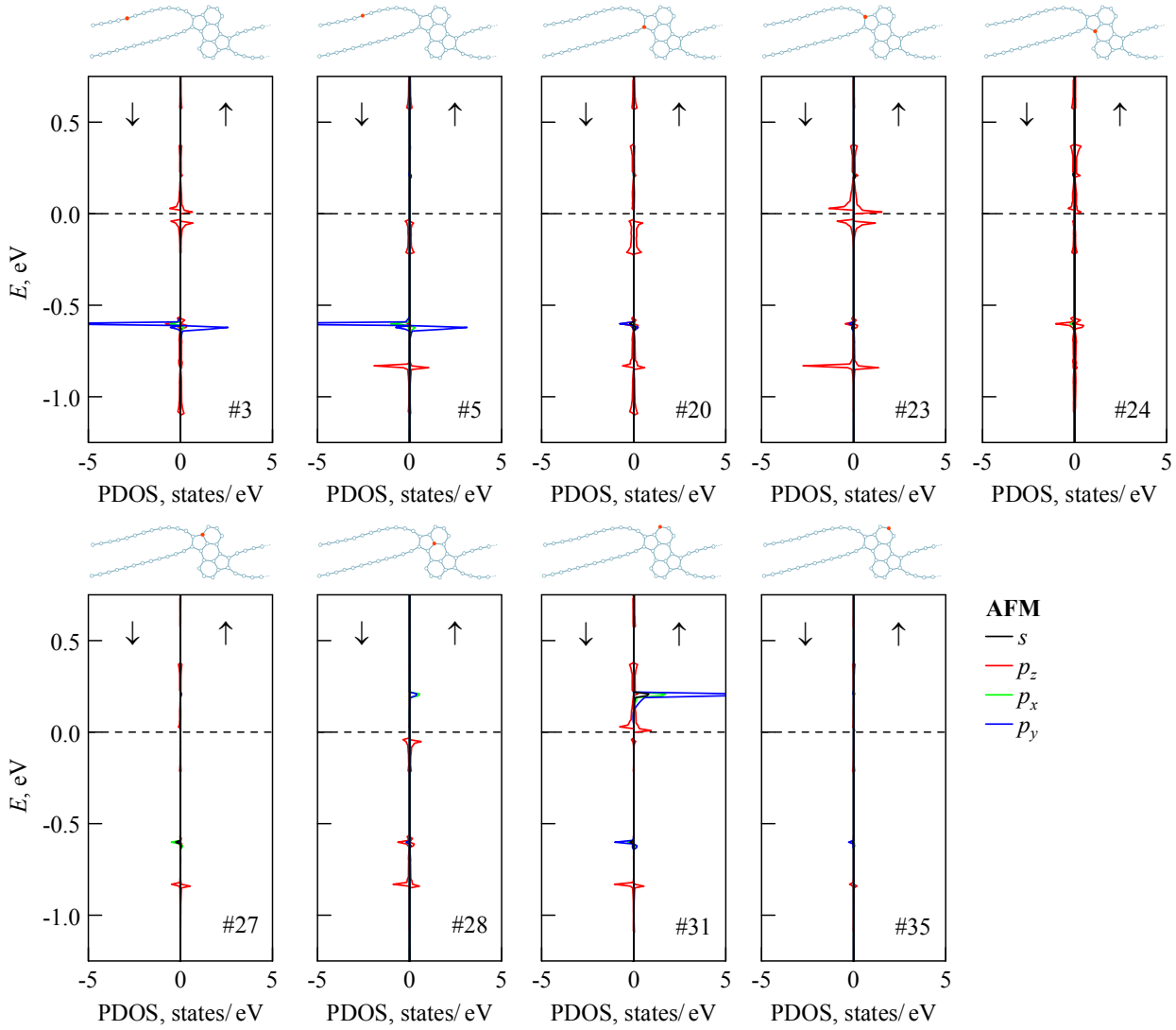
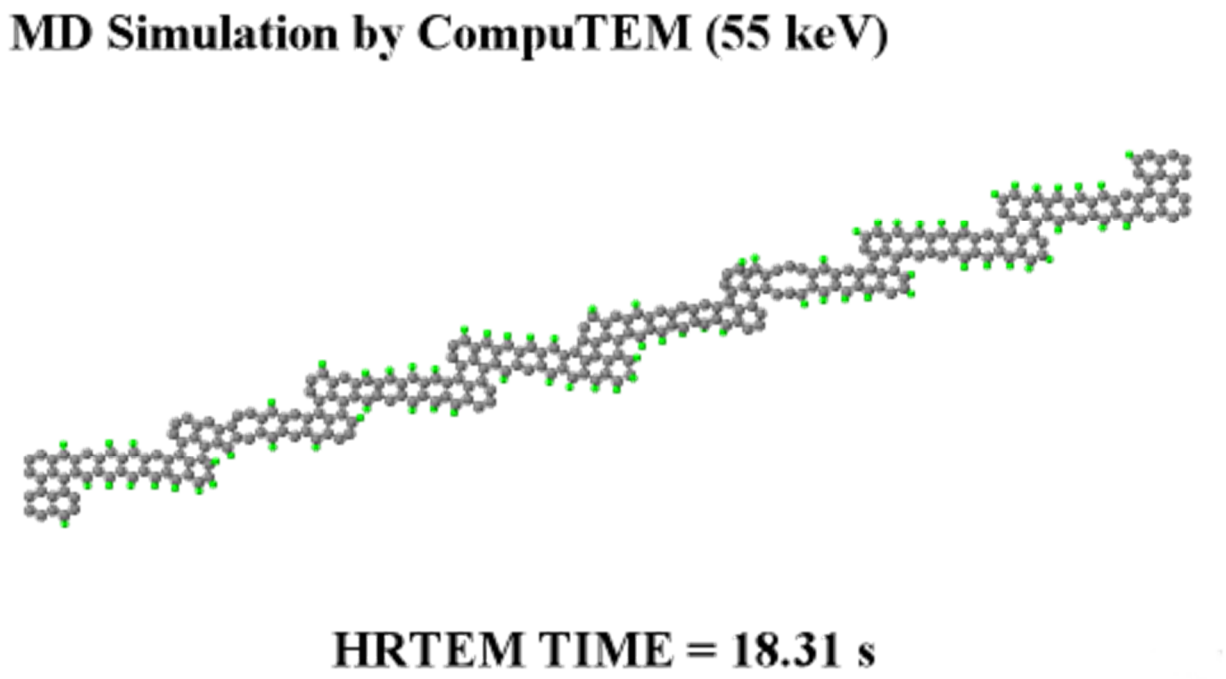


Figure S3. Calculated projected densities of states for selected atoms of the 1D nanoobject with D1 polycyclic regions (as indicated in the atomistic structures) in the antiferromagnetic state. The energies in eV are given relative to the Fermi level. The results for *s*, p_z, p_x and p_y orbitals are shown by black, red, green and blue lines, respectively.

Description of the video files attached

Video files "MD_SIMULATION_45keV.mp4", "MD_SIMULATION_55keV.mp4" and "MD_SIMULATION_80keV.mp4" show examples of the structure evolution observed in molecular dynamics simulations of the graphene nanoribbon transformation in HRTEM under electron irradiation with the electron kinetic energies of 45, 55 and 80 keV, respectively. In these video files, all carbon and hydrogen atoms are colored in grey and green, respectively. The total time in HRTEM (converted from the MD simulation time) is given at the bottom of the frame.



References

1. L. Ravagnan, N. Manini, E. Cinquanta, G. Onida, D. Sangalli, C. Motta, M. Devetta, A. Bordoni, P. Piseri and P. Milani, *Phys. Rev. Lett.*, 2009, **102**, 5502.

2. Z. Zanolli, G. Onida and J.-C. Charlier, *ACS Nano*, 2010, **4**, 5174–5180.