Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

HREELS Vibrational Signature of Graphene Nanoribbon edge topology

Nicola Cavani[1,2], Marzio De Corato[1,2] Alice Ruini[1,2] , Deborah Prezzi[2*], Elisa Molinari[1,2], Alberto Lodi Rizzini[1], Agnese Rosi[1], Roberto Biagi[1,2], Valdis Corradini[2], Xiao-Ye Wang[3] , Akimitsu Narita[3], Xinliang Feng[4], Klaus Müllen[3] and Valentina De Renzi[1,2*].

[1]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, I-41125 Modena, Italy

[2]CNR-NANO, Istituto Nanoscienze, Centro S3, I-41125 Modena, Italy

[3]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

[4]Center for Advancing Electronics Dresden (cfaed) & Department of Chemistry and Food Chemistry, Technische Universität Dresden, Mommsenstrasse 4, 01062 Dresden, Germany

*e-mail vderenzi@unimore.it, deborah.prezzi@nano.cnr.it

1. Supplementary Data

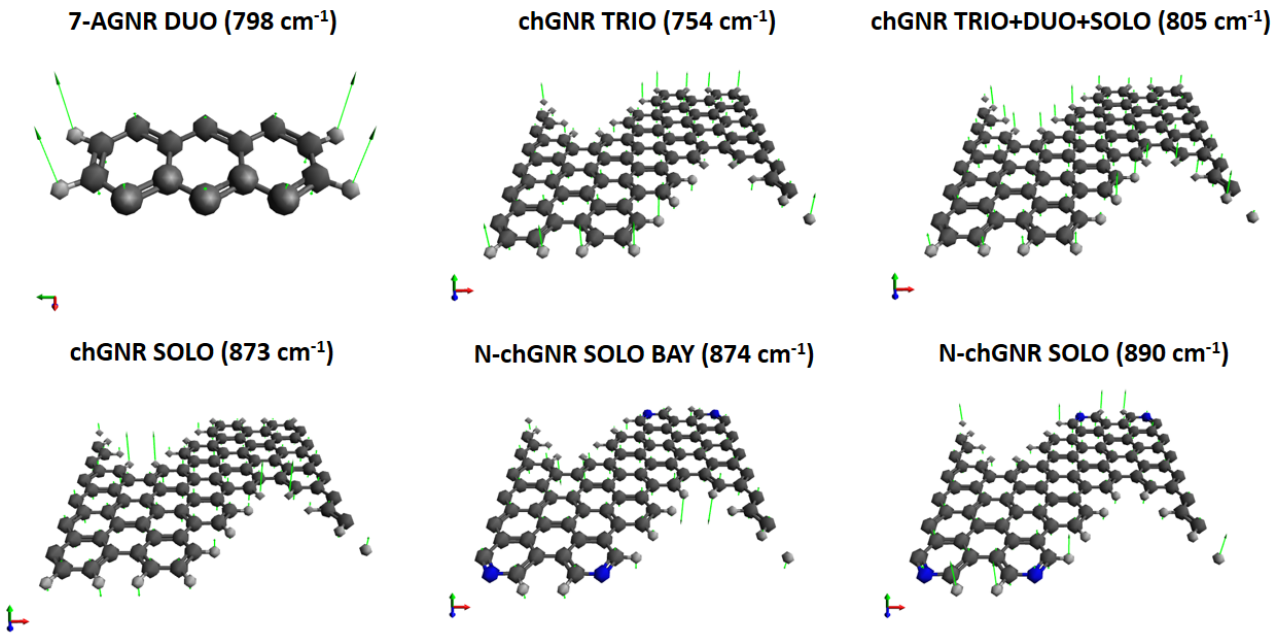

Figure S1 Selection of DFT-calculated atomic displacements for infinite 7-AGNR, chGNR and N-chGNR vibrational modes with their respective frequencies. Green vectors of different length represent the direction and the magnitude of the displacement for each atom involved in in the vibration.

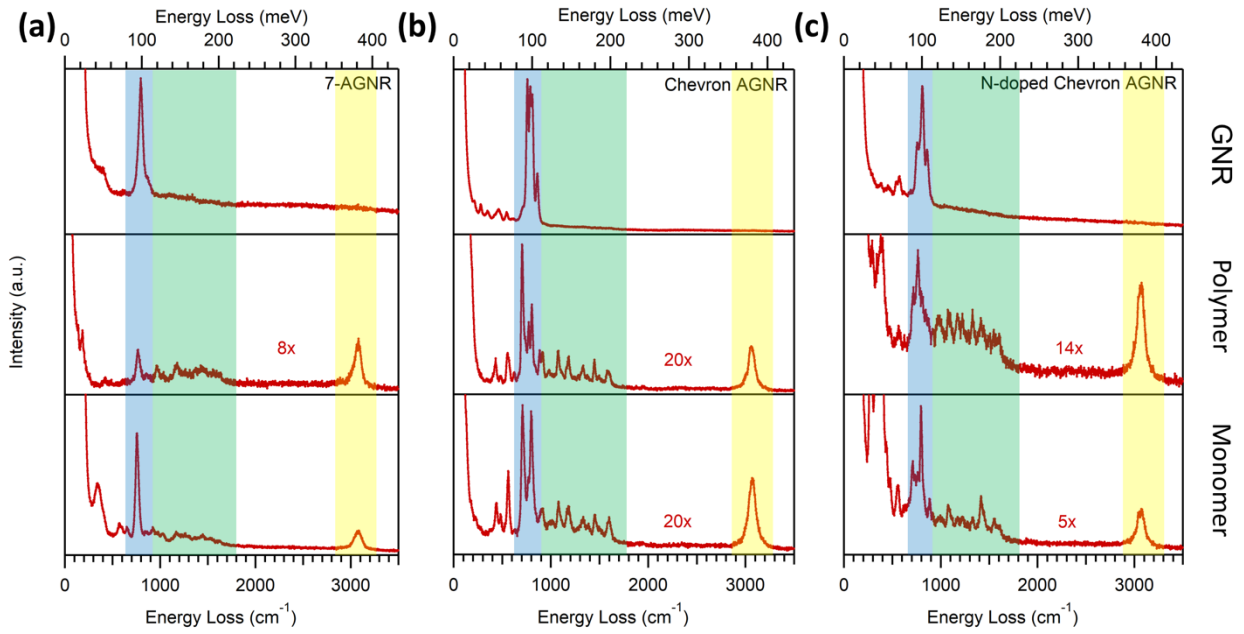

Figure S2 Vibrational spectra of the three main phases of GNR synthesis – i.e. monomer, polymer and nanoribbon – for 7-AGNR (a), chGNR (b) and N-chGNR (c). Different vibrational regions are highlighted with shaded colors: out-of-plane CH bending modes (wagging) with blue, in plane CH bending modes with green and CH stretching modes with yellow. Upon GNR formation, the molecular structure flattens, laying parallel to the surface. In this situation, both CH in-plane bending and stretching dipole modes oscillate parallel to the surface, thus becoming HREELS inactive. On the other hand, the intensity of out-of-plane CH bending modes hugely increases. The disappearance of the in-plane modes is therefore a clear fingerprint of the dehydrogenation step and can be used as a proof of the GNR formation, as first shown by Bronner et al.[1].

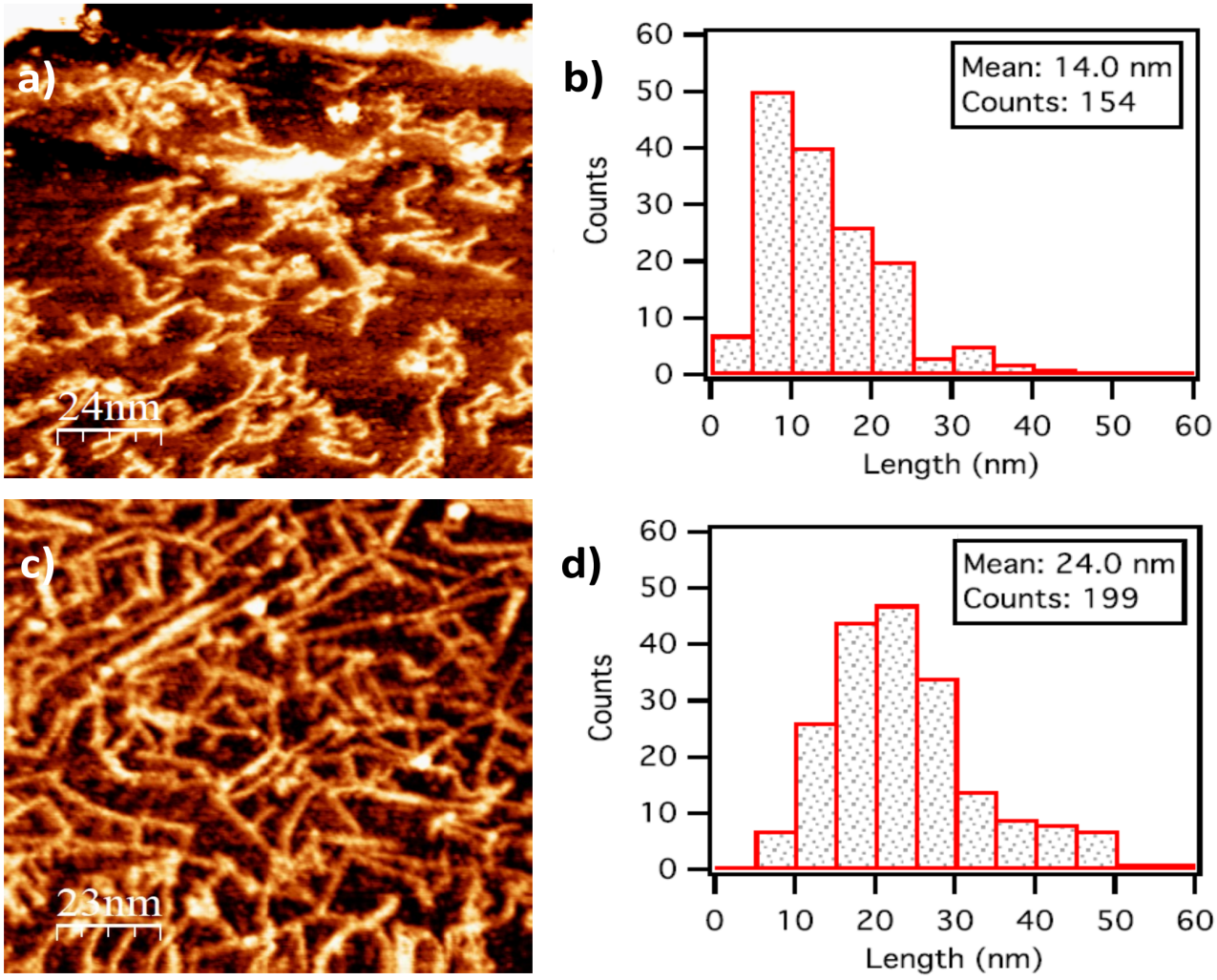

Figure S3 In (a) and (c) STM images taken at V= -0.25 V and I= 0.18 nA of 7-AGNR samples grown in different conditions – i.e. substrate deposition temperature T_D and coverage θ_{ML} – are displayed. The growth conditions are T_D = RT and θ_{ML} = 0.33 for the sample in (a) and T_D = 200°C and θ_{ML} = 0.26 for the sample in (c). In (b) and (d) the length distributions relative the images in (a) and (c) respectively, are reported. Though the area of the analyzed images is only 100 nmx100 nm, the histograms are fairly representative of the whole samples, providing clear indication that, on average, at T_D = 200°C longer GNR are obtained.

References

[1] C. Bronner *et al.*, "Aligning the band gap of graphene nanoribbons by monomer doping.," *Angew. Chem. Int. Ed. Engl.)*, vol. 52, no. 16, pp. 4422–4425, Apr. 2013.