Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Understanding the Electrochemistry of Armchair Graphene Nanoribbons Containing Nitrogen and Oxygen Functional Groups: DFT-calculations

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Figure S1: F. López-Urías et al.

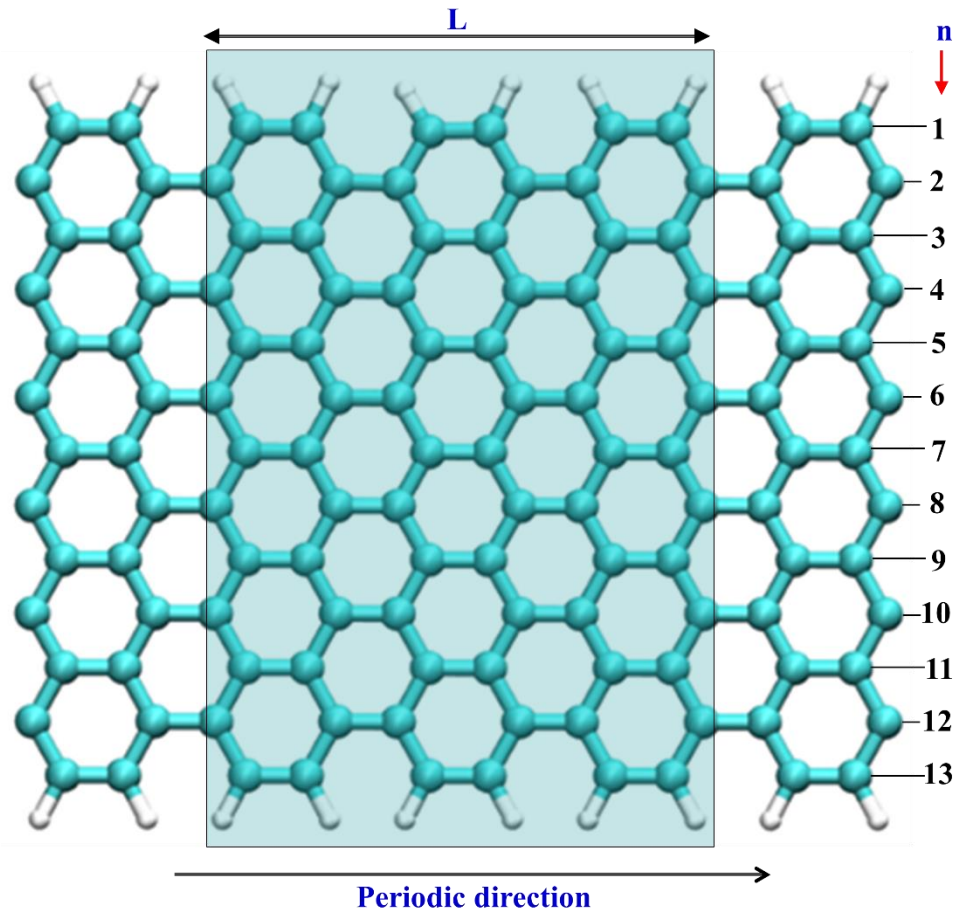

Figure S1: The geometry parameter of the supercell (shaded area) for the armchair graphene nanoribbon (AGNR). L refers to the length of the supercell and n labeling the carbon number along the zigzag chain. n=13 belong to the family of 3p+1 (p=4). The supercell contains 78 (12) carbon (hydrogen) atoms. The AGNR is periodic at the x-axis.

Figure S2: F. López-Urías et al.

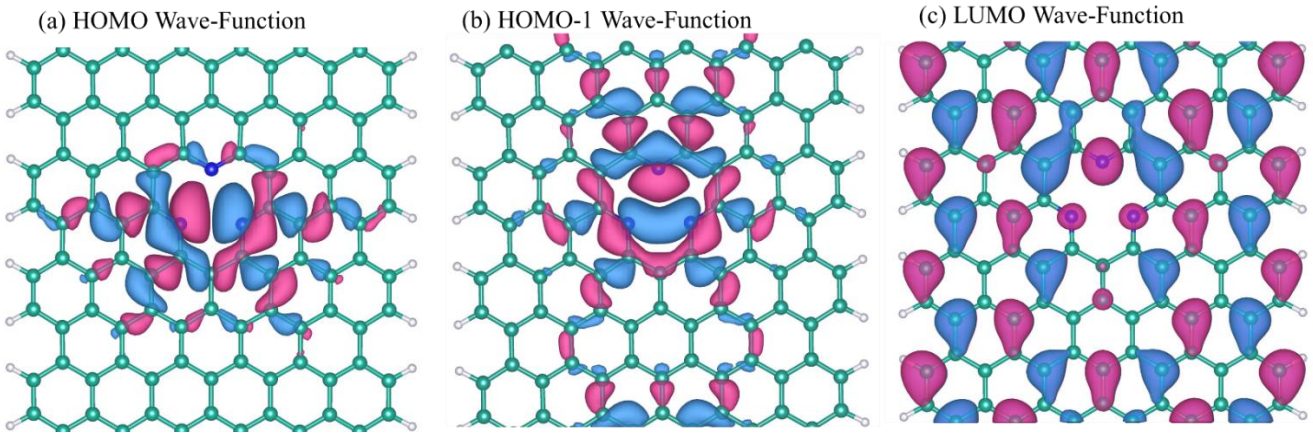

Figure S2: The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) wave functional calculated at gamma point of the N-pyridine doping AGNR. HOMO and HOMO-1 wave functions correspond to the energies of flat bands.

Figure S3: F. López-Urías et al.

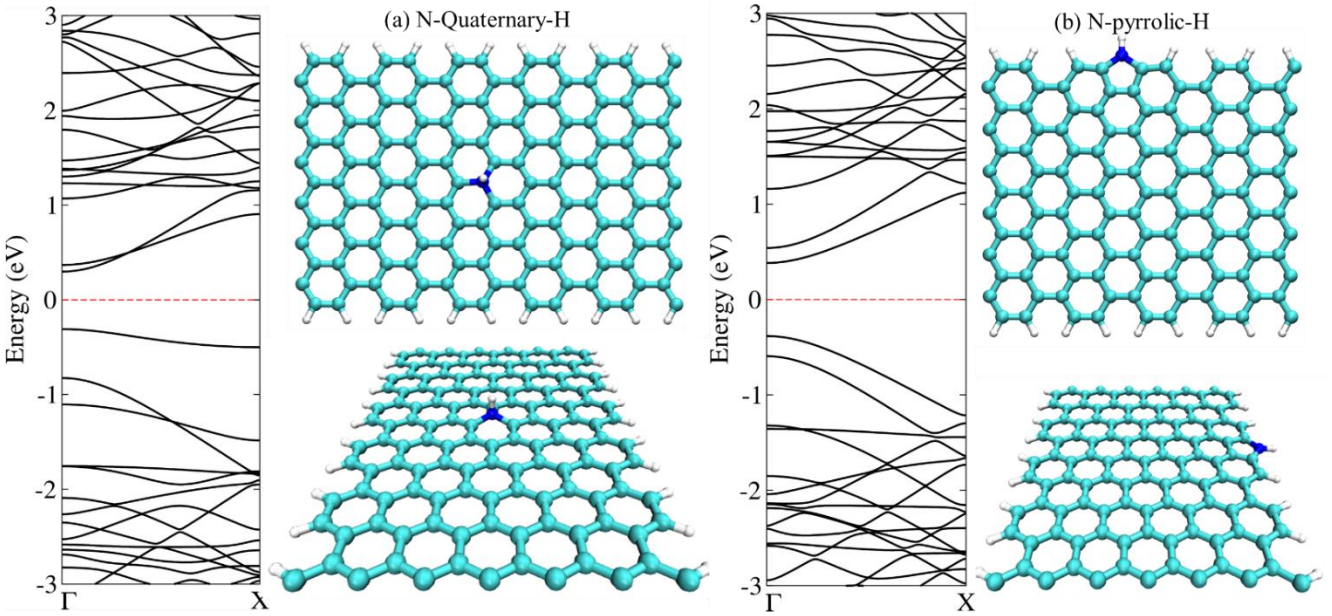

Figure S3: Band structure and the corresponding optimized structure for nitrogen doped AGNRs. **(a)** Hydrogenated N-Quaternary functional groups (N-Quaternary-H) and (**b)** Hydrogenated N-pyrrolic functional group (N-pyrrolic-H). A semiconducting behavior is obtained with an electronic band gap of 0.606 and 0.766 eV for N-Quaternary-H and N-pyrrolic-H, respectively.

Figure S4: F. López-Urías et al.

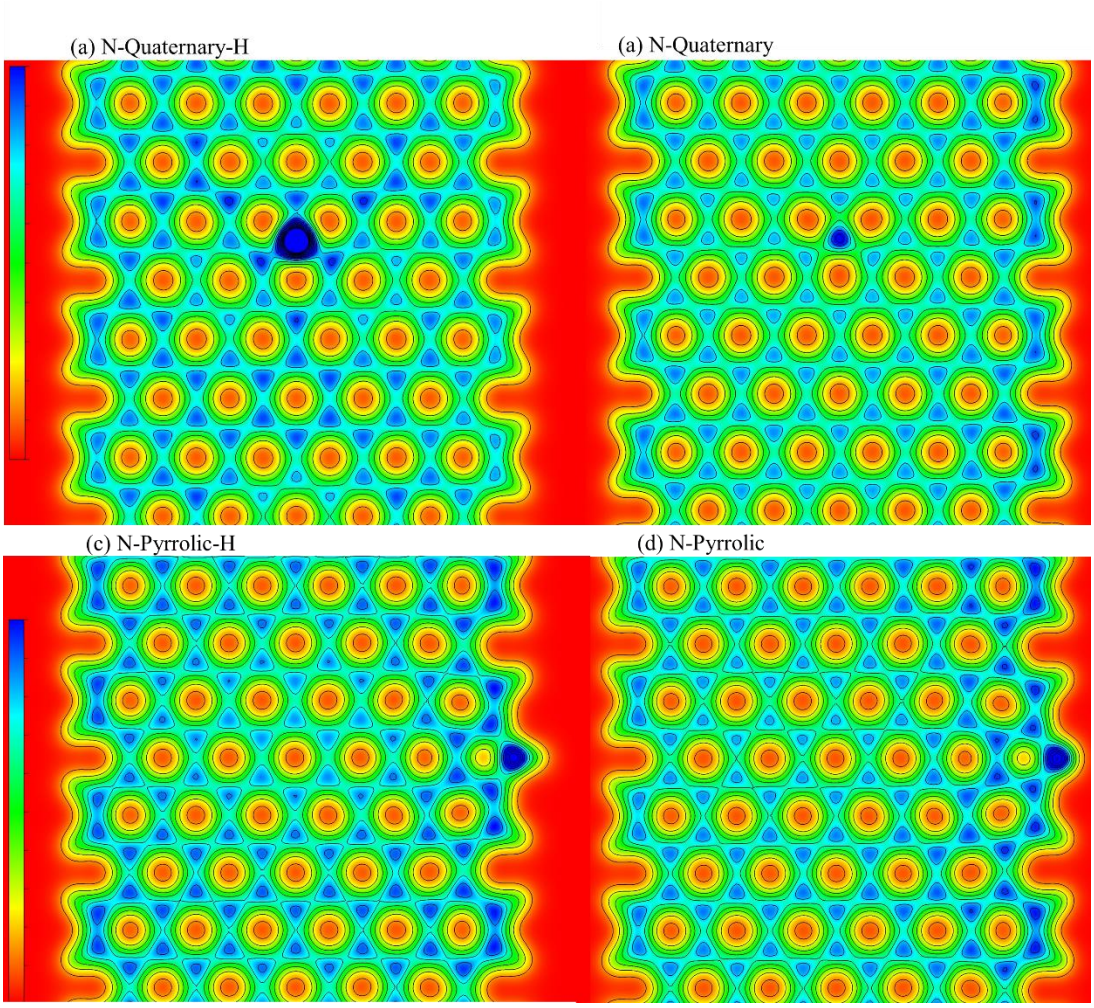

Figure S4: Charge density slide for **(a)** N-Quaternary-H, **(b)** N-Quaternary, **(c)** N-Pyrrolic-H, and **(d)** N-Pyrrolic. Low charge (red) and high charge (blue).

Figure S5: F. López-Urías et al.

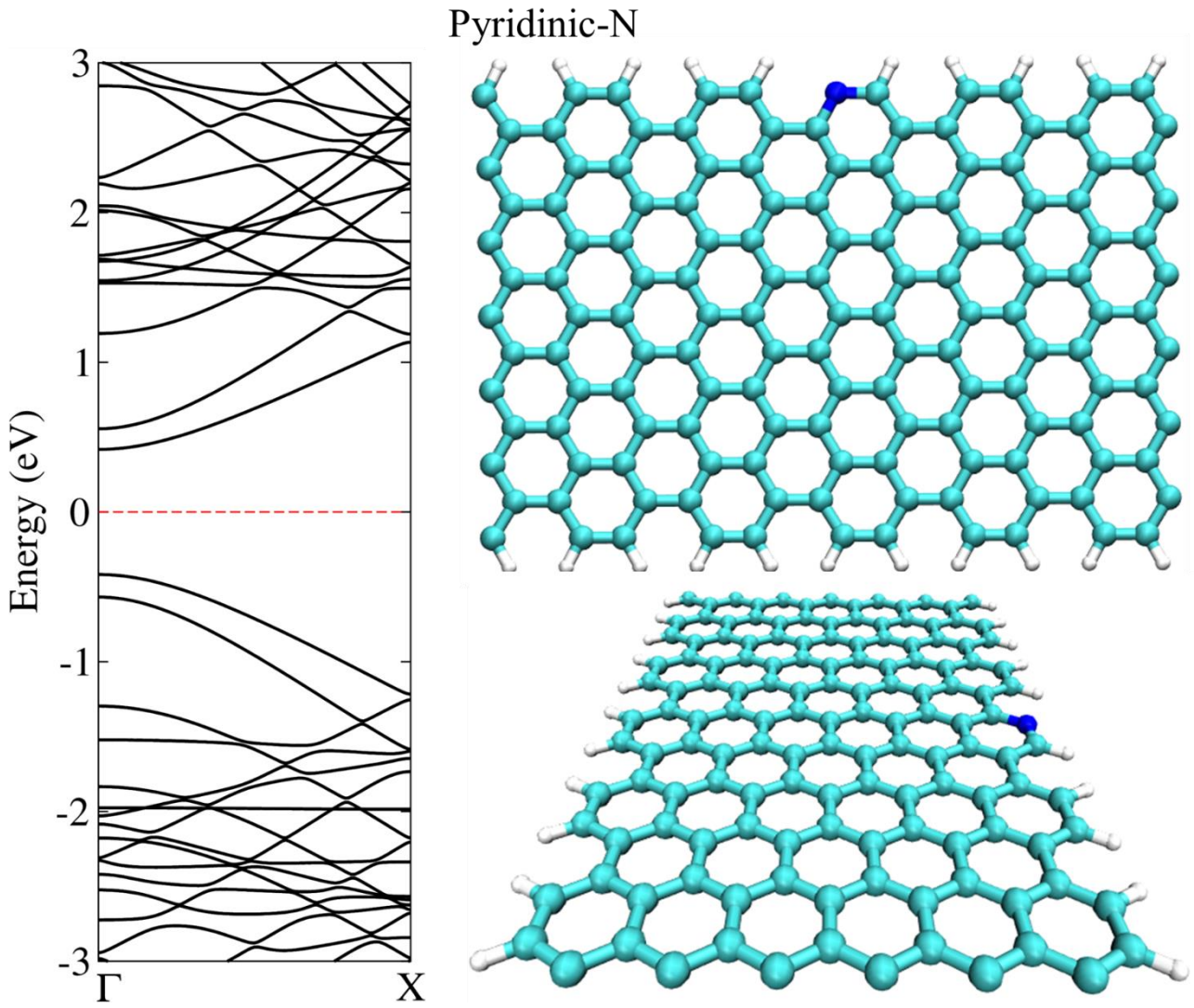

Figure S5: Band structure and the corresponding optimized structure (top and perspective views) for dehydrogenated pyridinium functional groups (pyridine-N) at the edge of the AGNR. The bandgap is of 0.835 eV.

Figure S6: F. López-Urías et al.

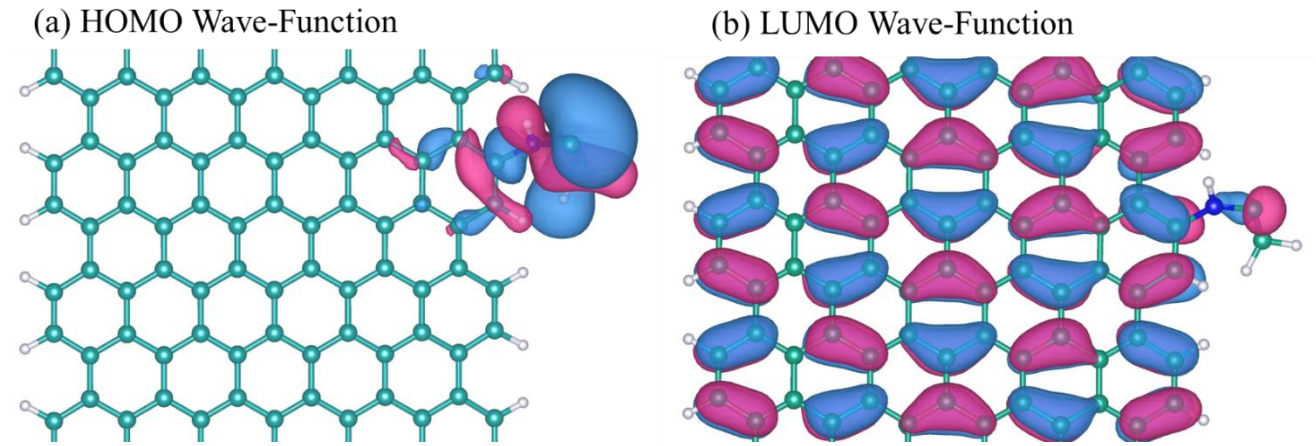

Figure S6: The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) wave functional calculated at gamma point of the N-ethylamine anchored to the edge of the AGNR. HOMO wave function corresponds to the energy of flat band.

Figure S7: F. López-Urías et al.

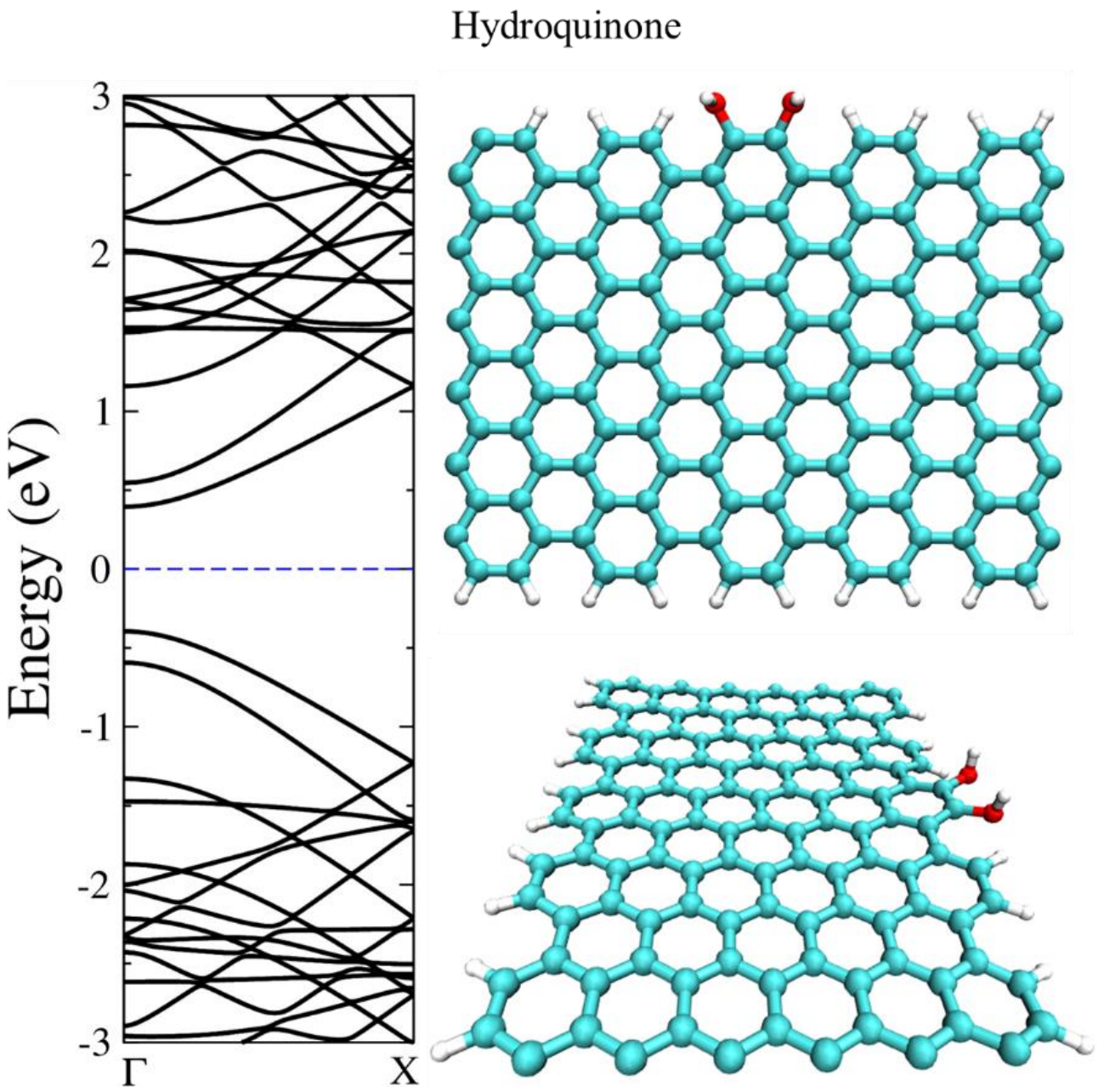

Figure S7: Band structure and the corresponding optimized structure (top and perspective views) for hydrogenated quinone group (hydroquinone) attached at the edge of the AGNR. The bandgap is of 0.789 eV.