Supplementary Information

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

Florentino López-Urías, Juan L. Fajardo-Díaz, Alejandro J. Cortés-López, Cristina L. Rodríguez-Corvera, Luis E. Jiménez-Ramírez, Emilio Muñoz-Sandoval

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.](image-url)
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: 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: 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: 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.

(a) HOMO Wave-Function  
(b) LUMO Wave-Function

**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.