

Furan and Pyran Functional Groups Driven the Surface of Nitrogen-Doped Nanofiber Sponges

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Highly surface oxidized, nitrogen-doped, and nitrogen functionalized carbon nanotube sponge (N-CFS) were produced at 1020°C using two sprayers approach in an aerosol-assisted chemical vapor deposition (AACVD) experiment. The structure of N-CFS consisted of entangled and corrugated carbon nanofibers of ~ 200 nm diameter, also showing junctions and knots. TEM characterizations revealed that the carbon nanofiber exhibits stacked graphitic layers in a transversal way with positive curvature. Superficial chemical analysis by XPS showed that the N-CFSs contain an atomic concentration of oxygen and nitrogen of 9.2% and 2.9%, respectively. The high-resolution XPS scans deconvolution-analysis revealed high percentages for C@O bonds, pyrrolic nitrogen doping, NH₃ functionalization, and Si@C interactions.

The cyclic voltammetry measurements did not display a redox process despite the high oxygen concentration at the surface. Hydrophobic functional groups containing C@O bonds do not participate in a redox process (furan, pyran, epoxy, methoxy, ethoxy, among others) could mostly determine the electroactivity of N-CFS. Based on density functional theory calculations, we determine that the furans transfer a high amount of electron and promote a positive curvature in thin carbon nanotubes. Graphitic materials with furans, pyrans, and epoxy functional groups could be used as an anode in lithium-ion batteries.

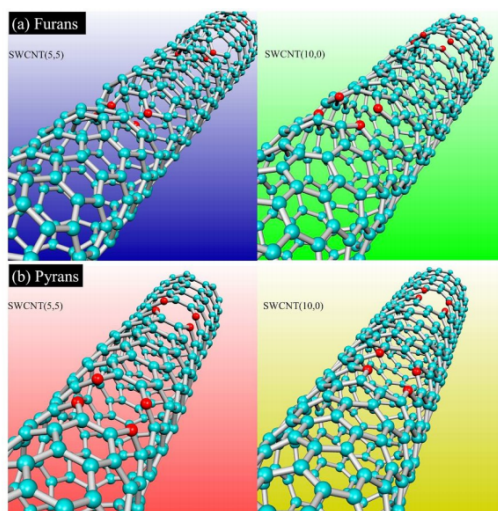


Figure 11. Relaxed structure of single-walled carbon nanotubes containing (a) furan and (b) pyran functional groups. Results for SWCNTs (5,5) and (10,0). Notice that the SWCNT (5,5) with furan functional groups exhibit positive curvature.