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

Supporting Information

Charge polarization in partially lithiated single-walled carbon nanotubes

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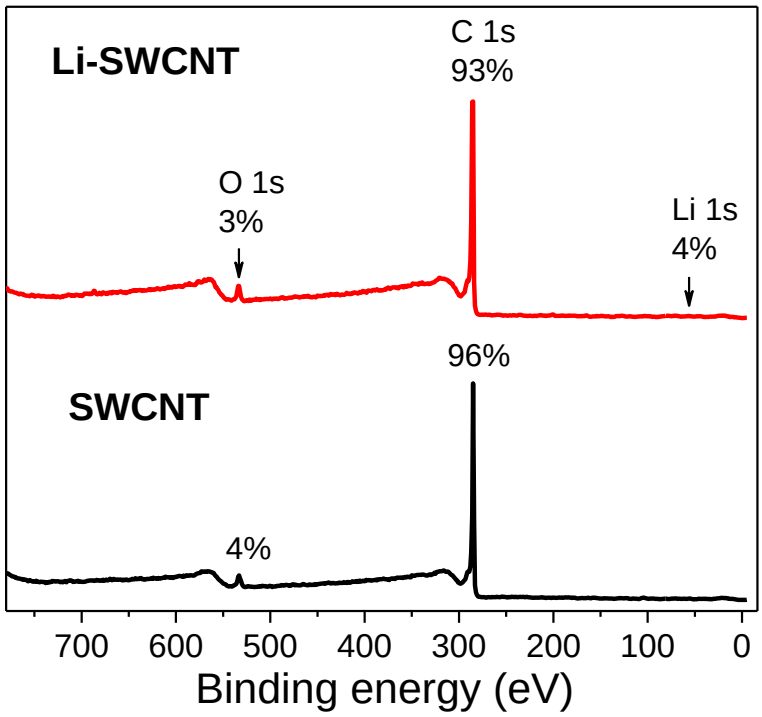

Figure S1. Survey XPS spectra of initial SWCNTs (bottom) and Li-SWCNTs (top) measured at an excitation energy of 830 eV.

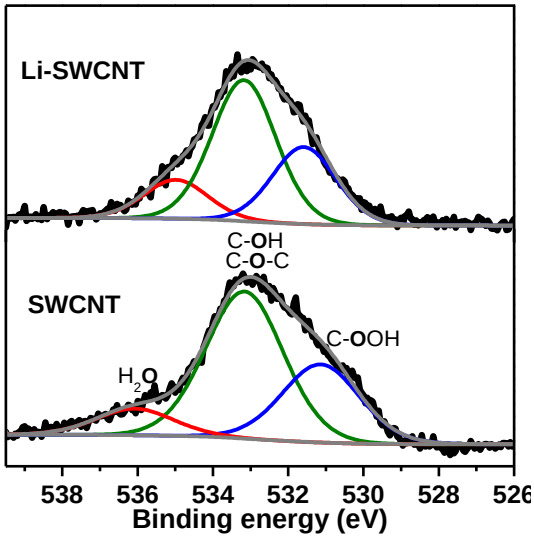

Figure S2. O 1s XPS spectra of initial SWCNTs (bottom) and Li-SWCNTs (top) measured at an excitation energy of 830 eV. The spectra were fitted by three components corresponding to oxygen atoms in H_2O, hydroxyl and epoxy groups, and in carboxyls.

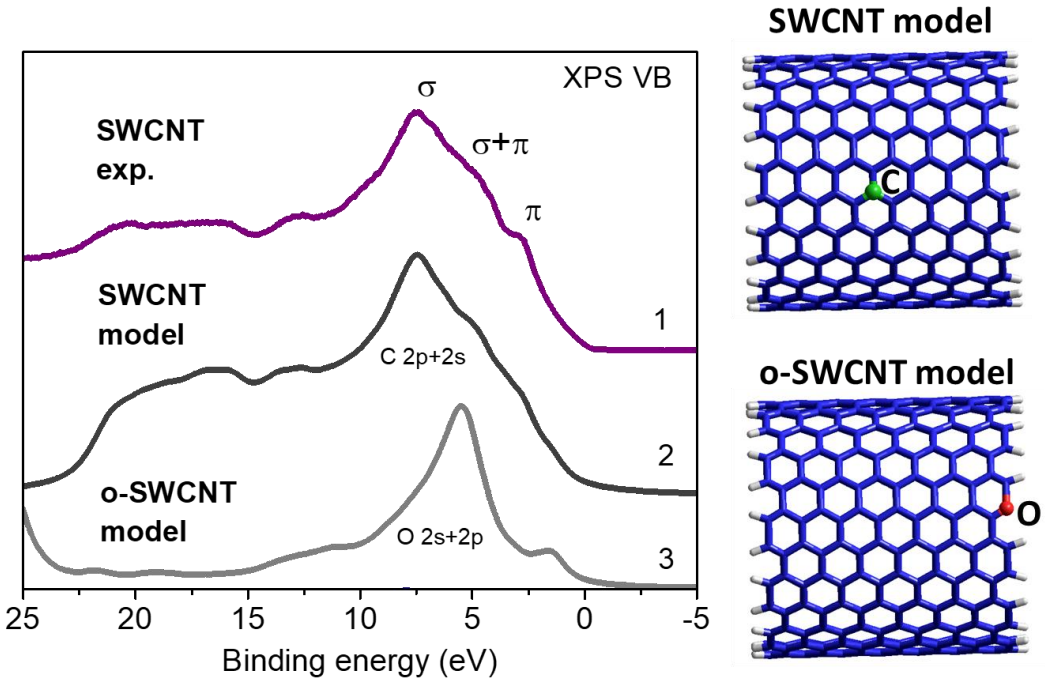

Figure S3. Experimental valence-band XPS spectrum of initial SWCNTs (curve 1) and theoretical spectra plotted for central carbon atom in the SWCNT model (curve 2, green C atom in fragment) and oxygen atom located at the edge of the o-SWCNT model (curve 3, red O atom in fragment). Intensities of the theoretical spectra are proportional to the density of occupied 2p and 2s states of carbon and oxygen atoms, without taking into account the concertation of atoms in models and atomic subshell photoionization cross-sections.

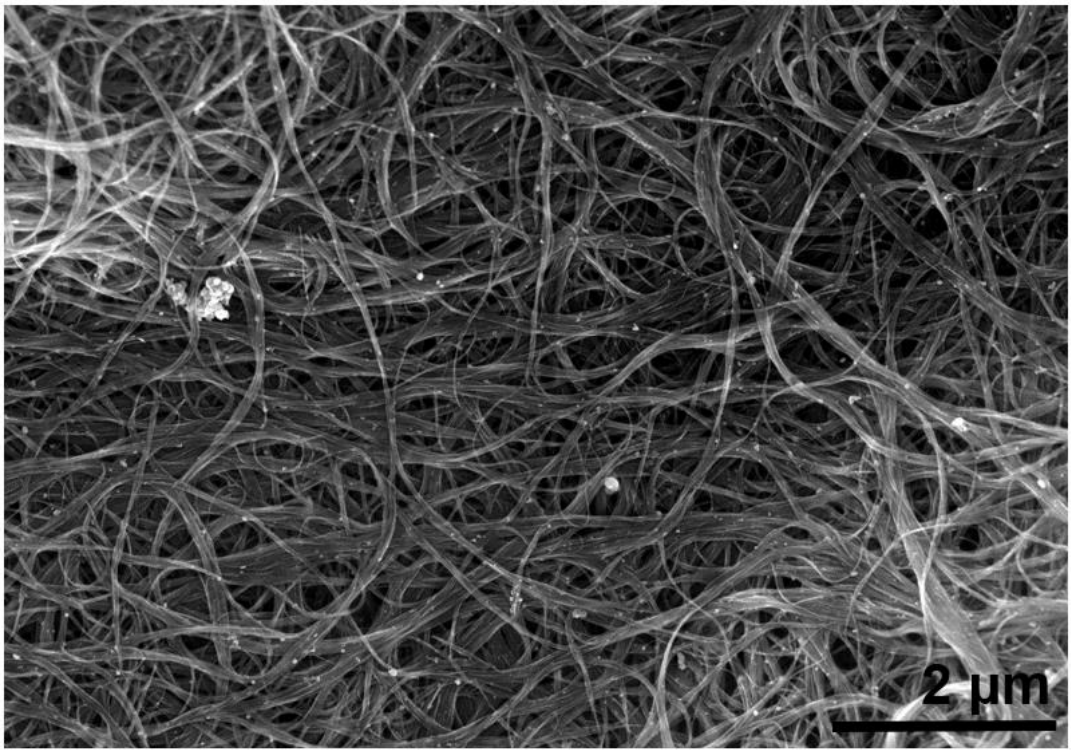

Figure S4. SEM image of SWCNTs with thermally deposited lithium. Bright dots, uniformly distributed in sample, most likely correspond to lithium nanoparticles.