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# The Influence of Oxygen Adsorption on the NEXAFS and Core-Level XPS Spectra of the C<sub>60</sub> Derivative PCBM

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Figure 1. O1s XPS calculated spectra of PCBM with one oxygen adsorbed to the fullerene cage on a 6-6 site (a) in the equatorial region of the cage and (b) in the vicinity of the side-chain. The arrows mark the peak being enhanced due to the presence of the additional O atom.

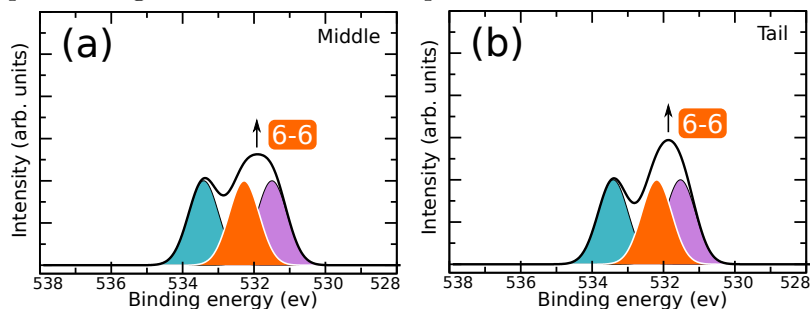


Figure 2. O1s XPS calculated spectra of PCBM with two O atoms adsorbed in the equatorial region of the fullerene cage: (a) both atoms on 6-6 sites and (b) one O on a 6-6, the other on a 5-6 site.

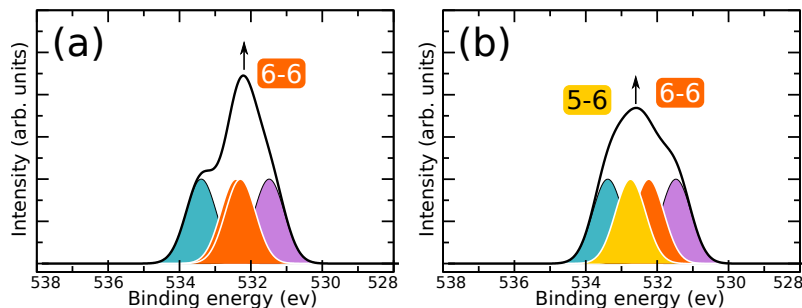


Figure 3. O1s XPS calculated spectra of PCBM with a singlet  $O_2$  molecule located at  $4 \text{ \AA}$  from the  $C_{60}$  cage, opposite of the side-chain.

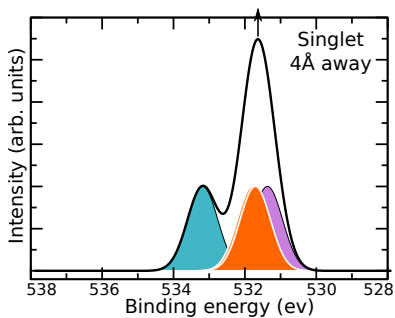


Figure 4. Calculated O1s NEXAFS spectra of PCBM with one oxygen adsorbed on a 6-6 site of the fullerene cage: (a) in the equatorial region and (b) in the vicinity of the side-chain. The arrows mark the appearance of additional peaks due to the adsorbed O atom.

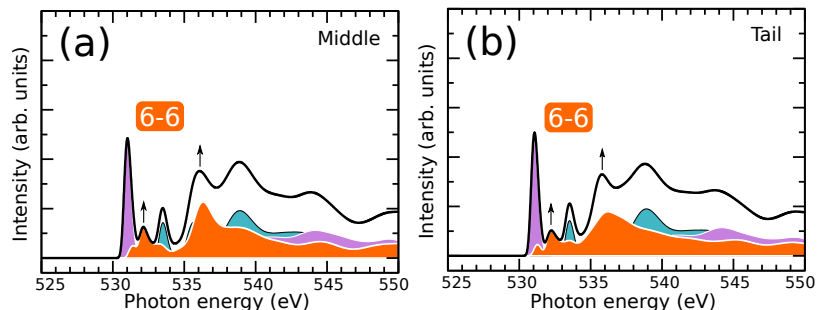


Figure 5. Calculated O1s NEXAFS spectra of PCBM with two O atoms adsorbed on the fullerene cage in its equatorial region: (a) both atoms on 6-6 sites and (b) one atom in the 6-6, the other in the 5-6 site.

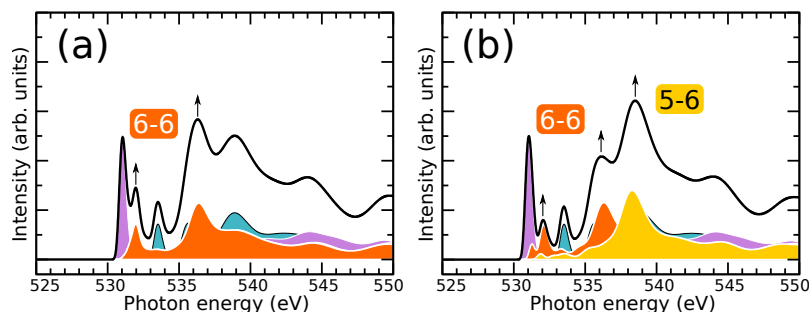


Figure 6. Calculated O1s NEXAFS spectra of PCBM with a singlet  $O_2$  molecule located at  $4 \text{ \AA}$  from the  $C_{60}$  cage, opposite of the side-chain.

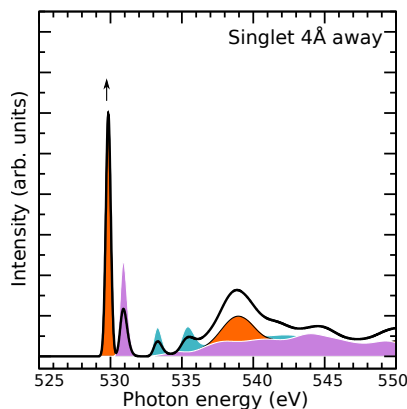


Figure 7. LUMO of the [6,6]-PCBM-O<sub>2</sub> (O<sub>2</sub> chemisorbed on a 6-6 site) in the presence of a half core hole on one of O atoms of the oxygen molecule. The orbital localization at the adsorption site is a core hole effect.

