The Influence of Oxygen Adsorption on the NEXAFS and Core-Level XPS Spectra of the C$_{60}$ Derivative PCBM

Iulia Emilia Brumboiu,$^{1, \text{a})}$ Leif Ericsson,$^2$ Rickard Hansson,$^2$ Ellen Moons,$^2$ Olle Eriksson,$^1$ and Barbara Brena$^1$

$^1$Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden

$^2$Department of Engineering and Physics, Karlstad University, SE-65188 Karlstad, Sweden

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$a)$Electronic mail: iulia.brumboiu@physics.uu.se
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 Å 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\textsubscript{2} molecule located at 4 Å from the C\textsubscript{60} cage, opposite of the side-chain.
Figure 7. LUMO of the [6,6]-PCBM-O\textsubscript{2} (O\textsubscript{2} 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.