Understanding PCBM's Unique Structural and Dynamical Properties through Computation and Experiment

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Phenyl-C61-butyric acid methyl ester (PCBM) is a fullerene-based material of great technological interest, due to its use as an electron-acceptor material in organic solar photo-voltaic cells (OPVCs). State of the art studies report that for devices with a thickness of 200 nm, PCBM and poly(3-hexylthiophene-2-5-diyl) blends can achieve solar-energy harvesting efficiencies of up to 10%[1]. One of the key factors for PCBM's success in such devices is its ability to optimise its structure and morphology through solvent and thermal annealing. This is something which has also been predicted from theory. Classical molecular dynamics studies have shown that the resultant structure of solid and amorphous PCBM differs drastically dependent on the thermal history and the temperature at which solvent extraction is performed[2]. Furthermore PCBM features a very rich behaviour regarding its thermophysical properties, notably the thermal conductivity of thin films is the lowest measured in materials with energy applications[3].

In order to devise a strategy to increase harvesting efficiencies, it is crucial that we gain insight into the structural and dynamical properties of PCBM. Fullerene based materials have previously been shown to have a very rich set of dynamical behaviours. In particular, fullerene itself was shown to undergo an order-disorder transition in the form of a rotor phase above 90 K[4]. We present quasi-elastic neutron scattering experiments that provide insight on such a transition in PCBM, as well as elucidating the collective mechanisms responsible for its ultra low thermal conductivity. Furthermore we perform classical and ab initio molecular dynamic simulations to gain microscopic insight into these phenomena and discuss the overall impact that this may have for the future manufacture of OPVCs.