

Performance of planar perovskite solar cells with mixed C60/C70 electron transport layer: an ab initio rationalization

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Planar perovskite solar cells have now achieved efficiencies on par with their sensitized counterparts. High performance planar perovskite cells utilize C60 as the electron transport layer (ETL) deposited using costly thermal evaporation. Recently, a mixed C60 and C70 solution-processed film with low crystallinity has been proposed as an ETL. The mixed-fullerene-based devices with a C60:C70 ratio of 9:1 achieved a similar or higher performance compared to their thermally evaporated C60 based counterparts.

Here, we present a density functional theory – density functional tight binding study of molecular and solid C60, C70, and the mixed system, aiming to rationalize these results. We show an excellent band alignment for electron transport of C60 and C70 components in solid state. The mixing energy of C60 and C70 components is computed to be on the order of kT at room temperature, implying absence of significant driving force to either segregation or desegregation. We also show a negligible effect of interfaces on the band structure. The computed electron transfer rates (using Marcus model) can be achieved with the C60/70 mixed structure are on the order of 10^{12} sec^{-1} , similar to pure C60.

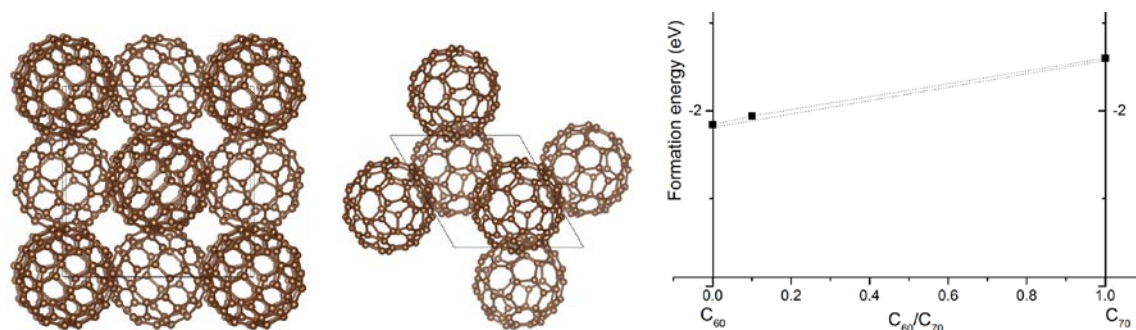


Fig. 1. Crystal structures of C60 (fcc) and C70 (hcp) as well as the convex hull for a mixed system with the C60:C70 ratio of about 10:1.

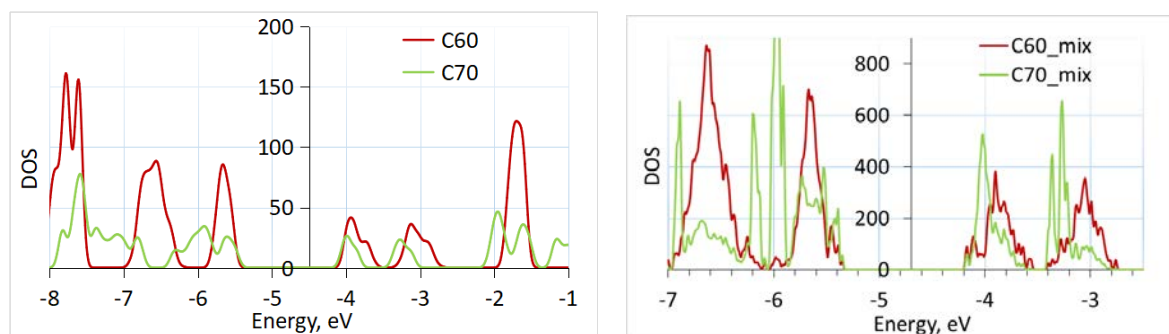


Fig. 2. Bandstructures. Left: of individual crystalline C60 (fcc) and C70 (hcp) crystals. Right: C60 and C70 components in a mixed system with the C60:C70 ratio of about 10:1.