Interplay between structural and electronic properties at Pb-free perovskite/electron transport material interfaces

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To cope with the toxicity issue of Pb-based perovskites and to achieve smaller electronic band gaps by alloying, Sn-based perovskites have gained growing attention recently [1–4]. Their surface and interface functionalization after assembling with electron transport layers (ETLs) are considered promising ways to pursue excellent optoelectronics and eco-friendly feature [5–7]. In view of the sophisticated chemical and physical properties of Sn-based perovskites, theoretical calculations based on density functional theory (DFT) have been employed to feasibly and flexibly model the interplay between absorbers and ETLs. In order to understand the fundamental physico-chemical mechanisms of that interplay, we have thoroughly investigated the influence of surface termination on structural and electronic properties at $FASnI_3/C_{60}$ (as ETL) interfaces, including intermediate work function calculations on free-standing slabs. The resulting type-II heterostructures coupled with the analysis of interface dipole moments and charge carrier mobilities allow predicting a spontaneous charge transport from $FASnI_3$ to C_{60}. Our findings contribute to discovering other promising alternatives as ETLs for lead-free perovskites in the light of surface and interface engineering.

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