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Influence of surface termination on electronic configurations at FASnI₃/C₆₀ interfaces

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Ever since organic-inorganic halide perovskites have been employed in electronics and optoelectronics, their unique and excellent photophysical and electrical properties[1–3] have guaranteed their versatile applications in solar cells, LEDs, lasers, photodetectors and beyond[4,5]. Sn-based perovskites along with their surface and interface functionalization after assembling with charge transport layers (CTLs) are considered promising ways to achieve a win-win between environmental friendliness and cell performance [6–10]. In view of the sophisticated chemical and physical properties of Sn-based perovskites, the theoretical calculation based on density functional theory (DFT) has been employed to feasibly and flexibly model the interplay between absorbers and CTLs. In order to understand the fundamental physico-chemical mechanisms of that interplay, the influence of surface termination on structural and electronic properties at FASnI₃/C₆₀ (as ETL) interfaces, in particular, the dependence of vacuum level (and by that work function) within surface alone and interface integrated frameworks, thereupon constructing the heterostructure energy level alignment, has been investigated thoroughly. The resulting type-II heterostructures coupled with the increased surface dipole moments and charge carrier mobilities tell an effective charge transport from FASnI₃ to C₆₀. 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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