Charge carrier dynamics across inorganic manganese perovskites and metal oxides interfaces

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Abstract

Inorganic perovskites are of high interest for perovskite cell applications in the recent years, due to their superior stability compared to mixed halide perovskites [1]. Previous research has shown that a replacement of toxic lead in the typical perovskite structure would in general lead to reduction of its performance, as with only a fractional substitution of lead with mercury were its properties marginally improved [2]. Several inorganic perovskites ($CaMnO_3$, $SrMnO_3$ and $BaMnO_3$) have shown promise for perovskite solar cell (PSC) applications due to their adequate band gap, and good optical properties, but also because they do not include lead in their composition [3]. Efficient device operation critically depends on the interface properties of the perovskite with neighbouring charge transport layers [4,5]. This study, based on first principles using density functional theory, focuses on the relevant properties which govern the charge dynamics at the interface of proposed manganite perovskite absorbers, and most popular electron transport layers (ETL) from the family of metal oxides (ZnO, TiO_2 and SnO_2). The relevant properties investigated within this work are electron effective mass, change in electronic properties of perovskites under strain, electrostatic potential, and relative band alignment. Because relative band alignment determines whether spontaneous charge diffusion occurs at the boundary of these materials, it is of vital importance for efficient operation of the PSC. Study reveals that the investigated perovskites grown on SnO_2 ETL have potential to be used in PSC. Most notably, $SrMnO_3$ and $BaMnO_3$ grown on SnO_2 have low lattice mismatch, which enables epitaxial growth, as well as optimal type II (staggered) band offset, which is crucial for spontaneous charge diffusion into ETL, and enables efficient operation of the device.

Keywords

Perovskite solar cells, manganates, charge dynamics, interfaces, density functional theory

References

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