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Title: Effect of surface capping ligands on excited state dynamics mediated via trap ststes in

C4cusb2cl12 layered double perovskites

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Abstract:

Perovskite solar cells recently emerged as one of the most promising photovoltaic technologies. Over a decade, the efficiency of perovskite solar cells enhanced from a meagre 3.8% to over 25.5%. They have progressed to compete with conventional crystalline solar cells in terms of both cost and performance. These solar cells offer facile synthesis methods, a tunable bandgap, and demonstrate the enormous potential to be used instead of silicon solar cells. In this regard, lead halide perovskites, particularly MAPbI 3, bring forth the most promising results. Despite unparalleled progress, lead halide perovskites to encounter several stability issues upon exposure to heat, oxygen, moisture and toxicity issues as they incorporate toxic lead. This has prompted researchers to explore other non-toxic and more stable substituents to lead halide perovskites for perovskite solar cells. The introduction of double perovskites (DPs) ushered in new possibilities for the development of stable and lead-free perovskites. In this respect, a new class of DPs namely Cs 4 CuSb 2 Cl 12 (CCSC) has been reported. CCSC has evolved to offer high photo and thermal stability and is tolerant towards stability. The suitable bandgap and higher conductivity of CCSC establish its potential as an absorber material for solar cell applications. However, the most pressing concern about CCSC is the presence of abundant surface traps which are detrimental to the stability and efficiency of the solar device. Here, to address this issue, we passivated surface traps using oleic acid (OA), oleylamine (OAm), and tri-octylphosphene (TOP) surface capping ligands. We used the UPS technique to determine hole trap states in CCSC. Moreover, we studied the excited dynamics of CCSC microcrystals (MCs) with and without capping ligands using femtosecond transient absorption spectroscopy.

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