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Theoretical spectroscopic investigation of hybrid halide perovskite solar cell materials

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Abstract:

Perovskite solar cells have recently become a very promising candidate in the search for an effective solar cell material. Over the past 10 years, their power conversion efficiency has increased to over 25% and there is a wide range of different potential chemical makeups that provide a range of materials to investigate. However, there are still questions about the specific role of all the different chemical components in the material. This thesis aims to investigate the effect of material composition and structure on the electronic structure of the system. Two largely separate investigations are presented: first a study on the differences between MAPI ($CH_3NH_3PbI_3$) and MAPB ($CH_3NH_3PbBr_3$) and how differences in local structure can affect the N 1*s* X-ray absorption spectrum. Various geometric parameters are found to affect the shape of the spectrum and these are explained via specific orbital changes. Second, charge transfer between the MA^+ ion and the inorganic PbI_3 lattice inside MAPI is investigated, and this is paired with an explanation of hybridization of states between MAPI and its Pb-less precursor MAI (CH_3NH_3I).

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