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First-Principles Investigations of Lead-Free Formamidinium Based Hybrid Perovskites ALTYNBEK MURAT, UDO SCHWINGENSCHLÖGL, PSE Division, KAUST, Saudi Arabia — Hybrid organic-inorganic perovskite solar cells have recently emerged as the next-generation photovoltaic technology. Most of the research work has been focused on the prototype $MAPbI_3$ perovskite (MA = Methylammonium = $CH_3NH_3^+$) and its analogues that have lead to power conversion efficiencies in excess of 15%. Despite the huge success, these materials are still non-optimal in terms of optical absorption where the bandgaps are greater than 1.6 eV as well as the toxicology issue of lead. Thus, investigation and development of lead-free perovskites with bandgaps closer to optimal, allowing greater spectral absorption, is of great interest. In this work, we perform first principles calculations to study the structural, optical, and electronic properties of new derivatives of $MAPbI_3$ in which the organic MA cation is replaced by other organic amines of similar size such as Formamidinium (FA) and/or the Pb cation replaced by similar elements such as Sn. In particular, we investigate the role and effect of FA and Pb cations on the electronic and optical properties and analyze to which extend the bandgaps can be tuned.

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