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Quantum-chemical calculations of lead-free perovskite materials on the basis of the density functional theory

Perovskites represent a modern and promising material for renewable energy sources. Since 2017, significant progress has been made with the further possibility of significantly improving the efficiency of perovskite solar cells. Moreover, the remarkable characteristics of hybrid perovskites as solar cell elements are mainly due to their excellent optical and electrical properties, such as a large absorption coefficient in the spectral region of ultraviolet radiation, high mobility of charge carriers, large diffusion lengths of electrons and holes, etc . The most well-known and widely studied hybrid perovskite system in photovoltaic applications is a type of lead halide such as lead methyl iodide iodide (MAPbI3, MA = CH3NH3) and lead formidium iodide (FAPbI3, FA = HC (NH2)2). These lead-halide perovskites are easily synthesized and have a low cost. However, their disadvantages are: chemical instability and toxicity; hybrid lead-halide perovskites contain heavy Pb atoms, which are poisonous and harmful. Thus, it is desirable to search for new hybrid lead-free perovskites containing non-toxic and available metals.

In this paper, calculations of several perovskite models in the form of CsBX3 and Cs2BB'X6 (where B and B 'are metals such as Pb, Si, Ge and Sn, X-halogen). The structural and energy characteristics of the systems CsSiI3, CsGeI3, CsSnI3, etc., were studied, in the presence of a "double" replacement of 2Pb <—> InBi, InSb, GaBi, etc. The possibility of using systems (Cs2SiGeI3, Cs2SiSnI3, ...) as candidate materials for environmentally friendly lead-free perovskite solar cells has been investigated. The DFT calculations are performed using the WIEN2k package, known methods of GGA-PBE and mBJ, where the main results of the analysis are the density of state (DOS) and energy characteristics.

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