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Computational Study on the Crystal Structure, Electronic and Optical Properties of Perovskites a2bx6 for Photovoltaic Applications

Authors : Harmel Meriem

Abstract : The optoelectronic properties and high power conversion efficiency make lead halide perovskites ideal material for solar cell applications. However, the toxic nature of lead and the instability of organic cation are the two key challenges in the emerging perovskite solar cells. To overcome these challenges, we present our study about finding potential alternatives to lead in the form of A2BX6 perovskite using the first principles DFT-based calculations. The highly accurate modified Becke Johnson (mBJ) and hybrid functional (HSE06) have been used to investigate the Main Document Click here to view linked References to optoelectronic and thermoelectric properties of A2PdBr6 (A = K, Rb, and Cs) perovskite. The results indicate that different A-cations in A2PdBr6 can significantly alter their electronic and optical properties. Calculated band structures indicate semiconducting nature, with band gap values of 1.84, 1.53, and 1.54 eV for K2PdBr6, Rb2PdBr6, and Cs2PdBr6, respectively. We find strong optical absorption in the visible region with small effective masses for A2PdBr6. The ideal band gap and optimum light absorption suggest Rb2PdBr6 and Cs2PdBr6 potential candidates for the light absorption layer in perovskite solar cells. Additionally.

Keywords : soler cell,double perovskite, optoelectronic properties, ab-inotio study
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