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First-principle study on the bandgap energy of MAPbI3

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Perovskite-type materials present different properties and applications in the field of technology such as solar cells, batteries and among others [1-2]. The organic perovskite of Methylammonium Lead Iodide (CH3NH3PbI3), also called MAPbI3, has been studied in this research to determine its bandgap by density of states (DOS) and band structure (BS) using the Quantum Espresso program.

[1] Bhalla A S, Guo R and Roy R 2000 The perovskite structure - A review of its role in ceramic science and technology Mater. Res. Innov. 4 3–26

[2] Li X, Zhao L, Yu J, Liu X, Zhang X, Liu H and Zhou W 2020 Water Splitting: From Electrode to Green Energy System Nano-Micro Lett. 12 1–29

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