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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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