

Temperature-Dependent Carrier Mobility in Methylammonium Lead Iodide

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Cubic methylammonium lead iodide (MAPbI_3) is one of the hybrid perovskite materials that exhibit high energy conversion efficiency for photovoltaics. Using Quantum Espresso, we calculate the energy profile of MAPbI_3 with the Methylammonium ion under different orientations within the cubic structure. Based on this energy profile we calculate the electron mobility as a function of temperature using the complex band method.