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Infrared spectrum and normal-mode assignment in methylammonium lead halide perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ MIGUEL ANGEL PEREZ OSORIO, MARINA FILIP, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK, CALLUM DOCHERTY, LAURA HERZ, MICHAEL JOHNSTON, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, UK, FELICIANO GIUSTINO, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK — Solar cells based on MAPbI_3 ($\text{MA}=\text{CH}_3\text{NH}_3$) have attracted enormous attention during the past two years owing to their high energy-conversion efficiency, reaching up to 19.3% in record devices. A detailed understanding of the structure/property relations of this compound may help us explain its extraordinary performance. Here, we investigate the vibrational modes and infrared (IR) absorption spectrum of MAPbI_3 by combining first-principles calculations and experiment. Our calculations indicate that the normal modes at high frequency, $400\text{--}3100\text{ cm}^{-1}$, correspond to internal vibrations of the MA cations, whereas those at low frequency, up to 180 cm^{-1} , can be assigned either to vibrations of the PbI network or to the libration and spinning of the cations. Using a factor group analysis we establish the symmetry of the normal modes and predict which mode will be IR or Raman active. In order to confirm these assignments we explicitly calculate the IR spectrum of the MAPbI_3 . The calculated spectrum is in good agreement with experiment, therefore we now have a complete characterization of the vibrational properties of MAPbI_3 . This work will serve as a solid reference for future structural and characterization studies of hybrid organic-inorganic perovskites.

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