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Phonon renormalization and anharmonicity in Al-doped MgB_2 FILIBERTO ORTIZ, RAMIRO QUIJANO, OMAR DE LA PENA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico., AARÓN AGUAYO, Facultad de Matemáticas, Universidad Autónoma de Yucatán, México. — We have studied the evolution of the E_{2g} phonon mode dynamics in $Mg_{1-x}Al_xB_2$ as a function of doping using the Frozen Phonon Approximation (FPA). The doping was modeled in the ab-initio Virtual Crystal Approximation (VCA). The results were obtained by means of first-principles total-energy calculations using the full potential Linearized Augmented Plane Wave (LAPW) method and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We present results for the evolution of the phonon frequency and anharmonicity of the E_{2q} mode as a function of Al concentration (x). From a comparison of the experimental data with the calculated E_{2q} phonon frequency we show that the VCA-FPA reproduces the observed phonon renormalization in the whole range of Al concentrations. More interestingly, we find that the anharmonicity gradually decreases with Al doping and vanishes for x(Al) > 0.5, that behaviour correlates with the evolution of the measured Raman linewidth in Al-doped MgB_2 . The significance of these results are discussed in the light of the experimentally observed loss of superconductivity in $Mg_{1-x}Al_xB_2$. This work was supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grant. No. 43830-F.

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