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Effect of magnetism on the electron-phonon coupling in iron-based superconductors LILIA BOERI, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany, MATTEO CALANDRA, CNRS and Institut de Minéralogie et de Physique des Milieux Condensés, case 115, 4 place Jussieu, 75252 Paris Cedex 05, France, OLEG DOLGOV, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany, IGOR MAZIN, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC 20375, USA — Phonons have been excluded as possible mediators for superconductivity in Fe pnictides based on early non-magnetic DFT calculations. However, it has later been argued that the lattice properties of Fe pnictides are better described by AFM calculations, with large moments. In this work, we calculate the effect of antiferromagnetic order on the phonon dispersion and electron-phonon coupling constant of $BaFe_2As_2$, using Density Functional Perturbation Theory. We show that the inclusion of magnetism increases the average electron-phonon matrix element by 50 % with respect to non-magnetic calculations. This is still not enough to explain the observed T_c in terms of e-ph coupling alone. We also show that the large magnetoelastic effects observed in FeBSC are not due to the electron-phonon coupling, but to the change in Fe-As bonding induced by magnetism.

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