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Large electron- A_{1g} phonon interaction in doped LaOFeAs: coupling with antiferromagnetism¹ FELIX YNDURAIN, JOSE SOLER, Universidad Autonoma de Madrid — We present first principles calculations of the atomic and the electronic structure of electron-doped LaOFeAs. We find that whereas the undoped compound has an antiferromagnetic arrangement of magnetic moments at the Fe atoms, the doped system becomes non magnetic at a critical electron concentration. We have studied the electron-phonon interaction in the doped paramagnetic phase. For the A_{1g} phonon, the separation between the As and Fe planes induces a non-collinear arrangement of the Fe magnetic moments. This arrangement is anti parallel for interactions mediated by As, and perpendicular for Fe-Fe direct interactions, thus avoiding frustration. This coupling of magnetism with vibrations induces anharmonicities and an electron-phonon interaction much larger than in the pure paramagnetic case. We propose that such enhanced interactions play an essential role in superconducting compounds close to an atiferromagnetic phase transition.

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Felix Yndurain Universidad Autonoma de Madrid

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