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Electron-phonon coupling in layered FeSe compounds[1]

TIMUR BAZHIROV, MARVIN L. COHEN, University of California, Berkeley — Iron-chalcogenide superconductors, showing many characteristic physical properties, can serve as a model materials to study the electron-pairing mechanism for all iron-based superconductivity. Layered iron-chalcogenide systems including single layer FeSe, bulk FeSe, K-intercalated FeSe, were studied using first principle pseudopotential density functional based approach. Electronic structure, vibrational properties and electron-phonon coupling strength were studied for the cases with and without iron magnetic moment ordering. The latter is incorporated using local spin density approximation. Our results show significant changes to electronic structure resulting in much higher electron-phonon coupling for spin-resolved configurations. Electron-phonon matrix elements for particular phonon mode of A1g symmetry are showing dramatic increase. Superconducting transition temperature estimates based on McMillan's equation are showing values significantly higher then previously reported, but still not high enough to account for the experimental results.

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