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A DFT+DMFT Investigation on Electron-Phonon Coupling in FeSe[1] SUBHASISH MANDAL, R.E. COHEN[2], Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C. 20015, USA, K. HAULE, Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA — The dramatic increase of superconducting temperature with external pressure in undoped FeSe has opened up a new route to investigate the mechanism of superconductivity. Using the self-consistent density functional theory-dynamical mean field theory (DFT-DMFT) method for paramagnetic FeSe as a function of compression, we find that there is greatly enhanced coupling between some correlated electron states between Γ and Z points and the A_{1g} lattice distortion. Except at high pressure, the maximum deformation potential in DFT for this mode is insensitive to increasing pressure, whereas the corresponding DFT-DMFT maximum deformation potential shows the same behavior with pressure as the experimental T_c, which first increases and then decreases with pressure. The Fermi surface average of the deformation potential in DFT-DMFT method can increase up to 50% when compared to standard DFT

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[2]& Department of Earth Sciences, University College London, Gower Street, WC1E 6BT, London, United Kingdom

Subhasish Mandal
Geophysical Laboratory, Carnegie Institution of Washington,
Washington D.C. 20015

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