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Electron-phonon coupling in C_{60} using exact-exchange functional
JONATHAN LAFLAMME JANSSEN, MICHEL CÔTÉ, Département de physique and Regroupement québécois sur les maériaux de pointe (RQMP), Université de Montréal, Canada — The superconductivity in C_{60} doped crystals is now well understood as a phonon mediated interaction. The strength of the electron-phonon coupling can be deduced by Raman and PES measurements which can then be used to assess the density-functional theory results. Although experimental and computed electron-phonon coupling agree on the total magnitude of the coupling, they do not on the contributions of the individual vibrational modes. Density-functional theory calculations indicate that high frequency modes are responsible for most of the coupling whereas experiments suggest that low frequency modes are the dominating contribution. Up to now, only calculations using the local density approximation (LDA) were performed. In this study, we investigate the effect of exact-exchange functionals, such as B3LYP, on the computed electron-phonon coupling of the different vibrational modes.

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