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Improvement of C_{60}'s calculated electron-phonon coupling using hybrid functional[1] JONATHAN LAFLAMME JANSSEN, MICHEL CÔTÉ, Département de physique and Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, University of California at Berkeley and Materials Sciences Division of Lawrence Berkeley National Laboratory — Superconductivity in doped C_{60} crystals is generally admitted to be phonon mediated. However, the electron-phonon coupling calculated within density functional theory do not agree with measured values, in contrast to others phonon related properties. This discrepancy hasn't been understood yet. Up to now, only calculations using the local density approximation for the exchange-correlation functional (LDA) were performed. In this study, we demonstrate that using exact-exchange functionals increases the calculated couplings, bringing it closer to experiment, while others properties, such as geometry and phonon frequencies, are little affected. We investigate how such an improvement is possible while little change is seen on more commonly calculated properties.

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