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Kohn anomalies and non-adiabaticity in doped carbon nanotubes

A. MARCO SAITTA, NICOLAS CAUDAL, MICHELE LAZZERI, FRANCESCO MAURI, IMPMC-Univ P et M Curie-Paris 6 — The tangential vibrational modes of metallic single-walled carbon nanotubes (SWNTs) are thought to be characterized by Kohn anomalies resulting from the combination of their intrinsic one-dimensional nature and a significant electron-phonon coupling. These properties are modified by the doping-induced tuning of the Fermi energy level ϵ_F , obtained through the intercalation of SWNTs with alkali atoms or the application of a gate potential. We present a Density-Functional Theory (DFT) study of the vibrational properties of a (n,n) metallic SWNT as a function of electronic doping. For such study, we use, as in standard DFT calculations of vibrational properties, the Born-Oppenheimer (BO) approximation, but we also use time-dependent perturbation theory to explore non-adiabatic effects beyond this approximation. We compare our results with existing measurements and suggest features to be explored in future experiments.

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