Strong effects of quantum anharmonicity on the structural and electronic properties of carbyne

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Recently, it has been shown how the correct treatment of quantum-anharmonic fluctuations (QAF) is crucial in the study of the phase diagram of many systems. Most relevant examples include superconducting hydrates, high pressure ice and even polymers like carbyne, an infinite-length straight chain of carbon atoms. In this latter system, DFT calculations show evidence of a competition between a second-order Peierls transition, mainly due to electronic contribution, and a first order phase transition whose role becomes relevant when QAF are included. In this work, I tackle the problem of carbyne's phase diagram using a toy-model with DFT-fitted parameters, including electron-phonon coupling. Despite its simplicity, the model allows to correctly reproduce first-principle-level calculations different from the one used for the fit, e.g. Born effective charges, and to include the effects of QAF in a fraction of the time usually needed, permitting to shed light on the properties of this polymer.