First-principles derivation of elastic interaction between Jahn-Teller centers in crystals via static lattice Green's functions

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Jahn-Teller (JT) systems with strong and intermediate vibronic coupling are described in terms of local JT active vibrational modes. In JT crystals, the elastic interaction of these modes at different JT centers plays a crucial role, for instance, in determining critical temperature of structural phase transitions. Despite their importance, the parameters of elastic interaction between JT centers have not been accessed yet by first-principles calculations. In this presentation, we describe a first-principles methodology for the calculation of elastic interaction parameters between local JT active modes of different JT centers in crystals. The method is based on the static lattice Green's functions which are obtained from the calculated phonon spectrum and polarization vectors of all phonon modes. As an example, the application of this methodology to the calculation of elastic coupling parameters in alkali-doped cubic fullerides A_3C_{60}, A=K, Rb, Cs, and double perovskites, $A_2BB'O_6$, based on heavy transition metals (B'=Os, Re, Ta, W), will be presented. The calculated elastic coupling constants in fullerides do not exceed a few meV, which supports the picture of non-hindered independent rotations of JT deformations in Cs_3C_{60} fullerides [1].

[1] Z. Huang, M. D. Albaqami, T. Sato, N. Iwahara, and L. F. Chibotaru, Phys. Rev. B. 103, 134102 (2021).