Quantum Anharmonic Effects on the Superconducting LaH_{10}

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The discovery of superconductivity in the H_3S at 203 K revived the attention on superconductors described through the Bardeen-Cooper-Schrieffer (BCS) and the Migdal-Eliashberg theories. Furthermore, the constant advancing of experimental and computational tools for the investigation and prediction of the system properties significantly widened the landscape on superconductivity in the BCS hydrides.

One of the most recent breakthrough is the discovery of the Lanthanum hydride (LaH_x) with a record superconductivity temperature of 250 K at a pressure of 170 GPa [1], [2]. The multiple experimental studies performed for this system reported different and distant values for its superconductive temperature (T_c) [1], [2], [3]. This suggests the existence of multiple superconductive phases coexisting at the same pressure. This feature sums up to the not yet well known stoichiometry of the material.

In this study we apply first-principle calculations including anharminic effects within the Stochastic Self Consistent Harmonic Approximation [4] (SSCHA) in order to accurately characterize the supeconductive properties of LaH_{10}. Our results suggest that the crystal structure of LaH_{10} is stabilized by quantum nature of the ions. This is similar to the situation in H_3S [5]. The superconducting properties and T_c are consequently strongly affected by large anharmonicity. Our results in LaH_{10} point again that quantum anharmonic effects are crucial in high-temperature superconducting hydrides.

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