

Lithium doping effects on electron-phonon properties of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

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The origin of unconventional high-temperature superconductivity in cuprate metal oxides is still a subject of ongoing research. Within the BCS theory framework and its generalization by Eliashberg, the introduction of high-frequency phonons, through methods such as doping light elements like lithium, can lead to stronger electron-phonon coupling and hence higher superconducting transition temperature. Drawing on these ideas, our study explores the effects of Lithium doping on the electron-phonon interactions in cuprates. We choose $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ (BSCCO, Bi-2212) as a prototypical cuprate and investigate how its structural, electronic, phononic and electron-phonon properties are affected by Li-Bi substitution. Full-Brillouin-zone electron-phonon calculations are highly time-consuming even with high-level parallelization. Here we present an economical method to calculate electron-phonon coupling, which has enabled an analysis on the atom, mode, and layer-resolved electron-phonon coupling for Li-Bi substitution.