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Electron-phonon coupling in A15 Cs₃C₆₀ and fcc alkali fullerenes

TAKASHI KORETSUNE, Tokyo Institute of Technology, SUSUMU SAITO — We study the electron-phonon couplings of alkali-doped fullerenes, fcc A₃C₆₀ (A=K,Rb) and A15 Cs₃C₆₀, using first-principles method based on the density functional theory. To improve the previous studies, we perform accurate calculations of phonon dispersion and electron-phonon coupling including momentum dependence and lattice symmetry. Furthermore, to estimate the superconducting transition temperature, we use Eliashberg equation instead of McMillan's formula. It is found that Eliashberg equation gives a quantitative improvement and that the obtained transition temperatures are reasonable compared to the experiments.

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