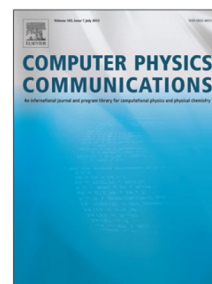


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Efficient method to calculate the electron-phonon coupling constant and superconducting transition temperature

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Abstract

We show an efficient way to compute the electron-phonon coupling constant, λ , and the superconducting transition temperature, T_c from first-principles calculations. This approach gives rapid convergence of T_c with respect to the size of the \mathbf{k} -point mesh, and is seamlessly connected to the formulation used in large molecular systems such as alkali fullerenes where momentum dependence can be neglected. Since the phonon and electron-phonon calculations are time consuming particularly in complicated systems, the present approach will strongly reduce the computational cost, which facilitates high-throughput superconducting material design.

Keywords: first-principles calculation, electron-phonon coupling, superconductivity

1. Introduction

Precise prediction of the superconducting transition temperature, T_c , and designing high-temperature superconducting materials are one of the ultimate goals for material design. Particularly for phonon-mediated superconductivity, several recent studies based on superconducting density functional theory

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