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Effect of Pseudopotential on Decomposition of Electron Phonon Renormalization

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ABSTRACT	Renormalization of band structure was obtained at zero temperature by electron phonon interaction and was called zero point renormalization. When temperature was increased then electron-phonon renormalization was increased due to occupation numbers temperature variations. Zero point renormalization of silicon was calculated. It was found that when temperature was high then band gap decreased. Results of electron-phonon interaction in case of silicon were made for different decay constants. Stability of overlap matrix was found. The band gap was reduced in lowest conduction band. It was also found that there was variation of decomposition of electron-phonon renormalization due to pseudopotential.

KEYWORDS	Renormalization, Occupation Number, Matrix, Band Gap, Pseudopotential, Adiabatic.

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INTRODUCTION

Giustino presented a mechanism for the study of electron-phonon interaction in solid [1]. Ponce et al., Karsai et al. and Miglio et al. studied the renormalization for small values [2, 3, 4]. Kune and Martin and Lam et al. used frozen phonon approach for the study of changes in band structure energies for phonon modes [5,6]. Monserrat used electronic solver for the study of supercell and their calculations considering adiabatic approximation [7, 8]. Allen and Heine used perturbation method for explanation of obtained results [9]. Expansion of electron potential was made. This was used for evaluation of integral, which respect to used samples density and was treated as interpolation schemes [10]. Gonze et al. presented computational effort using rigid-ion-approximation for the study of validity of approximation for study of validity of approximation on molecules and showed their contributions, which were less [11]. Antonius et al., Agapito and Bernardi and Lihm and Park

studied for which a way was used for improvement of perturbation based method and supercell based method [12-17]. Engel et al. calculated force constants which were used for the determination of phonon dispersion of a finite differences approach [18]. Matrix elements of electron-phonon coupling were used for finding Kohn Sham potential of first and second order. Calculations were made, using infinite differences approach. Louie, Giustino et al. presented that number of bands were used for convergence parameter evaluation and was calculated [19].

METHOD

Renormalization was calculated by first principle. Zero point renormalization of silicon was calculated for direct band gap. Efforts were made for improvement of perturbation based and supercell based methods. Strong localization were used for the study of Fourier interpolations. Born-Oppenheimer approximation was utilized for study of renormalization. Harmonic approximation was used for the study. Decoupling was given by the relation

$$\sum_{k'\alpha'} D_{k\alpha,k'\alpha'}(q)\, e_{k'\alpha',v}(q) = \omega_{qv}^2 e_{k\alpha,v}(q)$$

Where dynamical matrix is given by

$$D_{k\alpha,k'\alpha'}(q) = \sum_p e^{iq.Rp} \frac{\phi_{k\alpha 0,k'\alpha' p}}{\sqrt{M_k M_k^{'}}}$$

Where M_k is the mass of corresponding nucleus k, decoupled modes is given by $e_{k\alpha,v}(q)$, v_{qv} is the vibration frequencies index. Hamiltonian of phonons within harmonic approximation is given by

$$\hat{H}_p = \sum_{qv} \hbar\omega_{qv} \left(a_{qv}^{\dagger} \hat{a}_{av} + \frac{1}{2} \right).$$

All effects of electronic properties were studied. Final results of renormalization was found after making modifications from manybody theory. Density functional theory calculations were made for the study of electronic structure with the help of exchange correlation function. Parameterization of Perdew and Zunger of local density approximation was used. Bloch basis functions were given by the relation.

$$f_{\beta k}^{k}(r) = \sum_p e^{ik.T_{k,p}} \phi_{\beta k}(r - \tau_{kp})$$

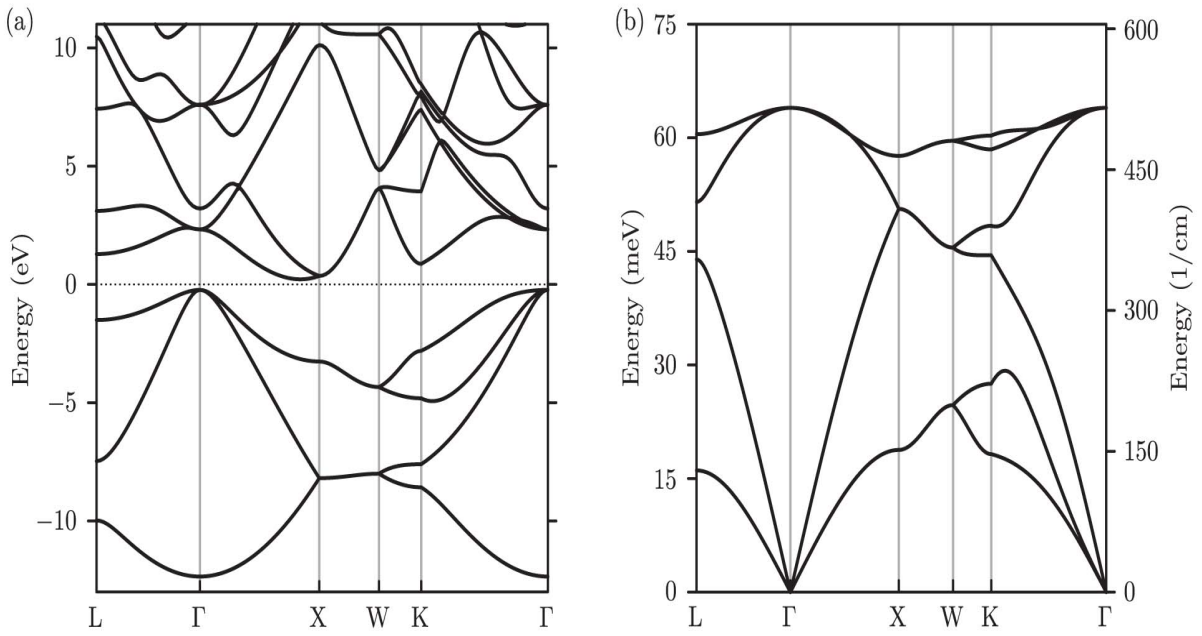
Where $\phi_{\beta k}(r - \tau_{kp})$ are localized Gaussian orbitals centered at τ_{kp}. Density functional theory wave function was presented by the relation

$$\psi_{nk}(r) = \frac{1}{\sqrt{N_{uc}}} \sum_{\beta k} c_{\beta k}^{nk} f_{\beta k}^{k}(r)$$

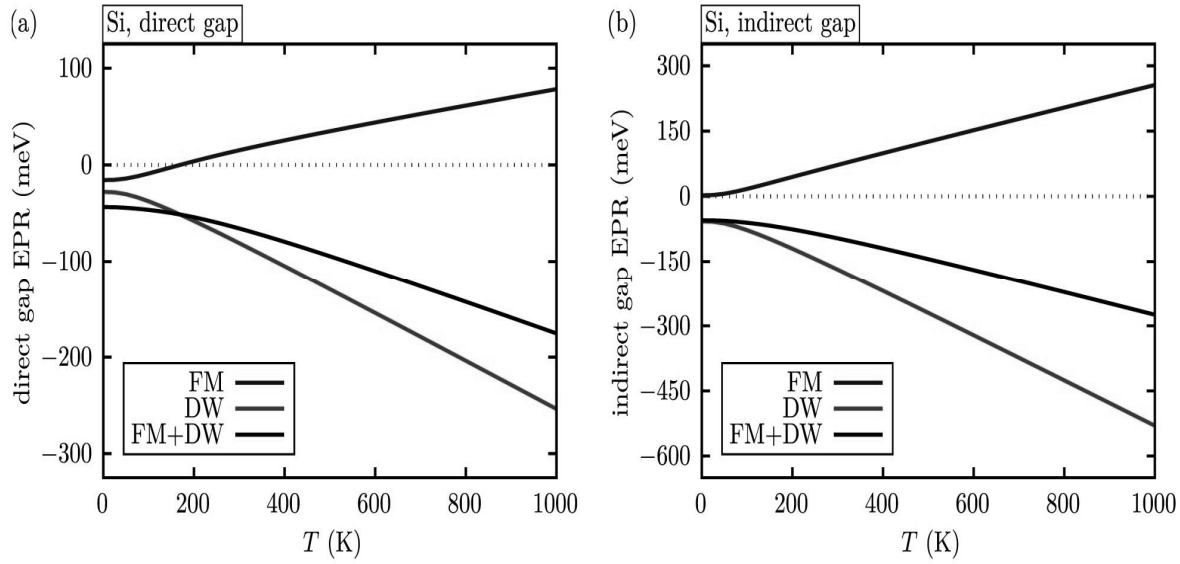
Where $c_{\beta k}^{nk}$ are coefficients force constants were calculated by phonon dispersion of finite differences approach. Matrix elements were obtained by wave functions of unperturbed atomic configuration. Electron-phonon calculations for silicon was made.

RESULTS AND DISCUSSION

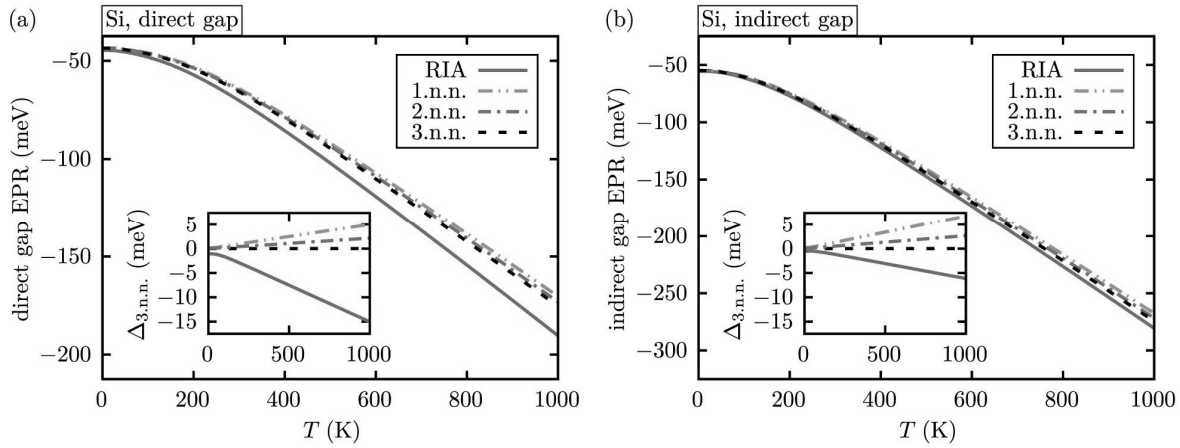
Renormalization of band gap was studied considering electraction between electrons and phonons. Graph (1) (a) shows band structure of bulk silicon. Graph (1)(b) shows the phonon dispersion of silicon. Graph (2) is plot of renormalization as a function of temperature. Graph (2) (a) and (2) (b) presents temperature dependence of renormalization. It shows that band gap is reduced due to increase of temperature. Two components of band gap was found as opposite dependence on temperature. Graph (3) (a) and Graph (3)(b) show contributions for different shells of nearest neighbors. First nearest neighbor provided slope of curve for direct gap was less deep. Shells of nearest neighbor contained a minor effect on slope.



Graph 1: Plot of band structure of bulk silicon vs electron phonon interaction.



Graph 2: Plot of renormalization as a function of temperature.



Graph 3: Plot of dependence of renormalization on temperature

CONCLUSION

Renormalization was studied by perturbation based Allen-Heine-Cardona method. Bulk silicon was considered for study of zero point renormalization was calculated for silicon. It was found that at high temperature, band gap shrinked. When temperature was increased electron-phonon renormalization increased due to occupation numbers of phonons. Efforts were made for improvement of perturbation based and supercell based methods. Final renormalization was found after making modifications provided from manybody theory. Matrix elements were evaluated by wave functions of unperturbed atomic configuration. Electron-phonon interaction calculations for silicon was made by using Gaussian having decay constants. It was found that the use of Pseudopotential affected the decomposition of renormalization for electron and phonons.

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