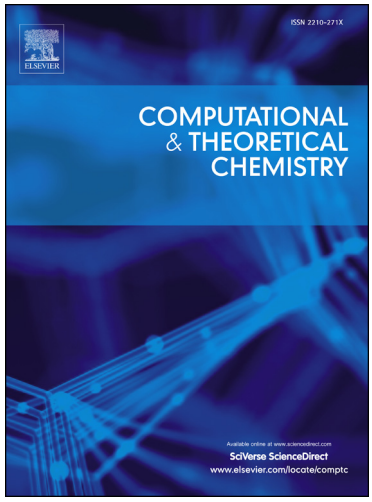

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Effect of long-range electronic correlation on exciton in the conjugated polymers

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[1]

Abstract

With the long-range electronic correlation Hamiltonian model, self-trapped exciton state in conjugated polymer under an electric field is investigated. It is found that the exciton binding energy is reduced by the long-range electronic correlation (LREC) effect compared to that without correlation situation, which means that the LREC effect is advantage for the exciton to dissociate into two quasi-particles: electron-polaron and hole-polaron. It is found that the LREC energy of the self-trapped exciton state has a bigger change when the applied field is over $4 \times 10^5 V/cm$ at which the self-trapped exciton has been dissociated into two charged-opposite polarons, that is, the LREC energy of the self-trapped exciton state is lower than that of two separated polarons state. It is also found that Hartree-Fock electron-electron (e-e) interaction reduces linear polarizability $\chi^{(1)}$ and third-order nonlinear polarizability $\chi^{(3)}$ of the exciton state, and the long-range electronic correlation effect furthers reducing $\chi^{(1)}$ and $\chi^{(3)}$.

Keywords: Self-trapped exciton; Long-range electronic correlation (LREC) energy; Correlation model Hamiltonian; Linear and nonlinear polarizabilities

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1 Introduction

Study of physical properties, such as electroluminescence, linear and nonlinear optical features[1][2], in organic polymers has been a much positive and hot field. Using these physical properties people can make chemical sensors, optically pumped lasers, light-emitting diodes, and photovoltaic cell devices and so on[3]. Due to instability of quasi one-dimensional lattice sites in organic polymers[4][5][6], there exists a special electron-hole pair state formed in a scope of one lattice site when an electron is excited by photo excitation or an applied electrical field from the top level of occupied molecular orbitals to the lowest unoccupied molecular orbital. This electron-hole pair state is so called self-trapped exciton state because that it is bound within a distorted lattice site[7][8][9]. The self-trapped bound exciton will be dissociated under stronger electrical field and has contribution to the optical process[10]. People have studied properties of one-exciton state and two-exciton state in the conjugated polymers under applied electrical field along the polymer chain direction[7][8] and also have studied polarizability of the single exciton[11][12] using tight-binding model. However, there is one very important factor that did not have been considered analytically in those studies about the exciton states and the polarizability. That important factor is the electronic correlation effect between π electrons. The electronic correlations usually are decomposed into strong (short-range) electronic correlation (on-site Hubbard

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