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Optical Response of Single Electron and Excitonic Systems in Carbon Nanotubes

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ABSTRACT

The study of optical response for single electron was made in the case of carbon nanotube using tight binding approach. The transitions between valence and conduction bands were calculated having interband linear susceptibility. The eigen values and eigen vectors were calculated using tight binding method. The interband response was found vanished for an ideal semiconductor at zero temperature. The long axis optical response along carbon nanotube chain axis was found. The transition for infinite periodic systems was observed. A realistic optical response of the system was calculated by applying many body effects in the system. The study of electron hole interaction by coulomb potential in the system was made. The calculation of excitonic effect for energies around the band gap was made. The Bethe-Salpeter method was used for calculation of excitonic effects for different systems having carbon nanotubes. The carbon nanotube chain system was considered for the study of optical response of excitonic system. In this case electrons and holes were located on the same subsystem. The exciton states as linear combinations of electron and hole band states in the conduction and valence bands were considered. The band structure of the system showed the encapsulation of the chain inside the carbon nanotube made the sub systems intact with each other. The interaction affected the electronic structure of the system and produced band gap. The changes in the electronic structure created changes in the single electron and also optical response of the system due to optical transitions. The obtained results were found in good agreement with previously obtained results.

KEYWORDS

Optical Response, Tight Binding, Transition, Susceptibility, Eigen Vector, Excitonic Effect, Band Gap Interaction.

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INTRODUCTION

Wang et al. [1] and Wisman et al. [2] studied experimentally the optical response of different single walled carbon nanotubes. Spataru et al. [3] Maultzsch et al. [4] and Hiu et al. [5] calculated the optical response and exciton binding energies for different carbon nanotubes and found exciton binding energy around 0.4 eV. Dukovic et al. [6] and Jiang et al. [7] presented that the binding energy depended on the structural characteristics of the carbon nanotubes and also on surrounding materials. Miyauchi et al. [8], Deslippe et al. [9] and Ando [10] studied the effect of coulomb screening of electron and holes for carbon nanotubes. Zhao et al. [11] presented that structure problem was solved by encapsulating inside multiwalled carbon nanotube. It was shown that the most stable carbon chain has single and triple bond lengths of 1.329 and 1.229 Å were grown for longer inside double walled carbon nanotubes with an optimum distance of 3.38 Å between the chain and carbon nanotube [12]. Mostanni et al. [13] studied the optical linear response for exciton and excitonic gap for polyenes using a simplistic model of one π orbital persite. Vander Horst et al. [14] and Pedersen [15] made excitonic calculations using Bethe-Salpeter method and exciton binding energies of 0.2 – 0.9 ev for different kinds of polymers consistent with experimental data. Burteaux et al. [16] and Sun et al. [17] showed that the electronic structure and optical properties were different for isolated systems and it was followed a similar trend like for encapsulation of carbon chains inside the carbon nanotubes. Shi et al. [18] studied the encapsulation down shifted the band gap energy of carbyne in comparison to carbon chains such as finite polymers and excitonic effects on the optical response of carbon nanotube chain systems were calculated. The exciton binding energy energies were also calculated. Gonze et al. [19], Bottin et al. [20] and Torrent et al. [21] studied the electronic structure using density functional theory and ABINIT package having the Perdew-Burke-Emzerhof generalized gradient approximation to obtain eigen states of the system. Lanzillo et al. [22] presented the tight binding band structure, when it was fitted with density function theory for carbon nanotube chain system and band gap was calculated for the chain band and corresponded transitions. The quasi particle correction opened the (8,0) carbon nanotube band gap to 1.8 ev and the chain band gap was found 2.58 to 4.71 ev which depended on the strain of the chain [23]. The tight binding was used to calculate the linear optical response of the system was studied by Bonabi and Pedersen [24] and interband linear susceptibility for different transitions. Tomio et al. [25] studied the suppression for stronger and excited states for reduction of binding energies. Wagner et al. [26] studied the strain dependent electronic structure and optical properties of an (8,0) carbon nanotube using cutting edge. The physical properties studied were used for emerging applications. It was found that the optical absorption spectrum was highly strain dependent. Forster et al. [27] studied the properties of carbon nanotubes and mechanical behavior dominated due to stiffness and large rapture strain and were found chemically very stable. Wagner et al. [28] showed that the sizable shift of electronic energy levels as a function of axial strain and this shift presented optical transitions sensitive to strain.

METHOD

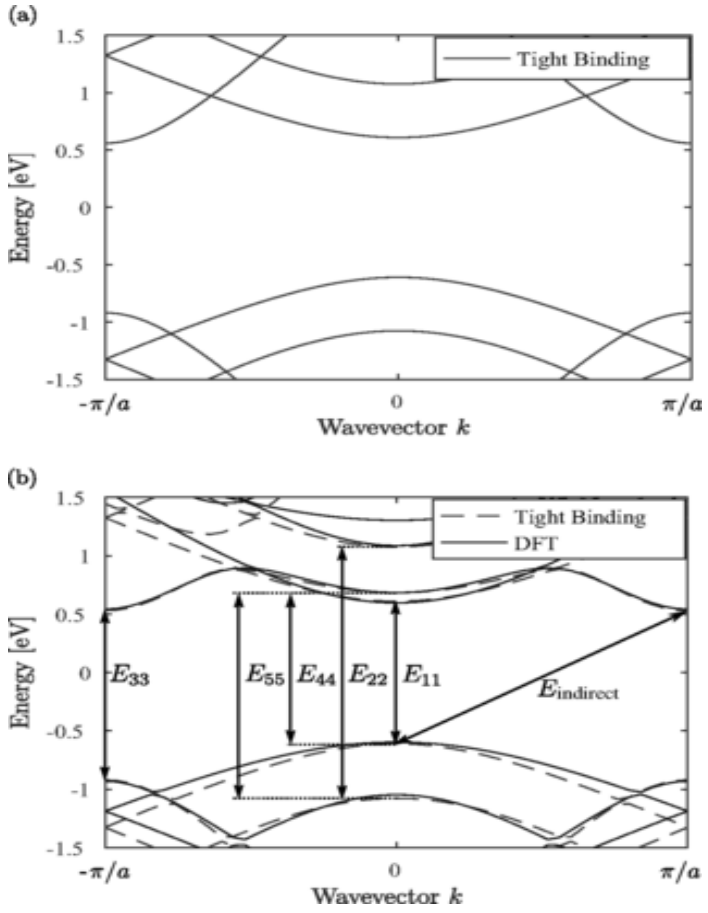
For calculating the optical properties of the system we have calculated the band structure of the system applying tight biding approach using density functional theory for band structure of the combined system was affected due to interaction of two isolated systems. The bond length of carbon nanotube and length of unit cell for carbon nanotube was obtained. The single and triple bond lengths of carbon in chains were calculated. The separation between the carbon nanotube and the chain having carbon-carbon distance in each system was calculated. The electronic structure of the system was described by π-orbitals in carbon nanotube and chain. The hybridized eigen vectors were used for the computation of matrix elements. The effective masses of electrons and holes in high symmetric points of Brillion zone and adjustable tight binding parameters were used for obtaining effective masses. The tight binding method was used for calculation of linear optical response of

the system. The transition between valence and conduction bands for periodic system of interband was observed. The difference of energy between conduction and valence bands were calculated. The eigen values and eigen vectors were calculated from the tight binding approach and broadening was found. In the case ideal semiconductor having temperature of zero degree and zero electrostatic field the interband response vanished. The long axis optical response along the carbon nanotube chain axis were considered for the study. The excitonic optical response of the system was calculated by taking into account many body effects in the system. The electron-hole interaction through coulomb potential in the system was considered. The calculation of excitonic effect for energies around the band gap using two different approaches were made. The Bethe-Salpeter method was used for the calculation of excitonic effects for different systems. For obtaining excitonic optical response the carbon nanotube chain system was used. It was found that electrons and holes were located at the same system. The matrix kernel was determined by the electron-hole coulomb interaction in an exciton basis. The integration was performed using electron and hole band states. For dark excitons the dominant contribution was momentum difference between the electron and hole band states. The bare coulomb potential was obtained through interaction between π-atomic orbitals of electrons and holes and was approximated by Ohno type potential. The screening of the problem was made. Wannier model provided a reasonable accuracy and was modified on a set of approximations. Exciton states was calculated using Schrodinger like equation in Hartree units.

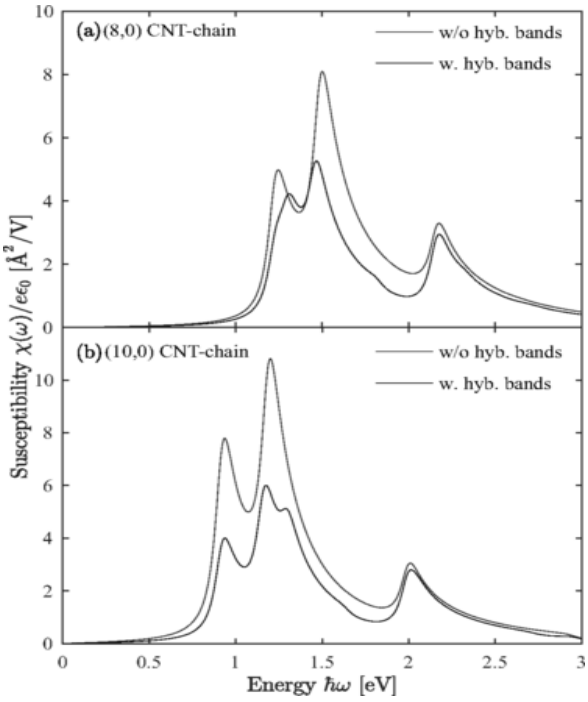
RESULTS AND DISCUSSION

For the calculation of optical properties the band structure of the sytem was calculated using tight binding approach and compared with the obtained results of density functional theory band structure. The electronic structure of the system was described by taking π-orbitals for carbon nanotube and chain. For obtaining band structure of the combined system the hybrized selected bands of the carbon nanotube and chain were considered. Graph (1) (a) shows the tight binding structure of the isolated system having Fermi energy at O ev. Graph (1) (b) shows the tight binding band structure with density functional theory for carbon nanotube chain system. The density functional theory calculation provided 0.62 ev for the (8,0) carbon nanotube band gap and 0.88 ev for the chain band gap corresponding to transitions E_{11} and E_{33}. A scissors shift of 0.6 ev to open the density functional theory band gap and was found in good agreement with tight binding band structure. Graph (1) (a) and Graph (1)(b) show the dominant part of the band structure comes from the isolated systems. Graph (2) shows the optical responses and single electron linear susceptibility for (8,0) carbon nanotube chain system and (10,0) carbon nanotube chain system with and without band hybridization. The optical response for isolated carbon nanotubes and chains were found. The interaction between the carbon nanotube and chain were calculated for single particle optical response for the combined systems. The obtained results showed that band hybridization had significant effects on the single electron optical response. The Bethe-Salpeter model was used to calculate excitonic effects on the optical response for the system of different parts of the electrons and holes. Graph (3) (a) and (3) (b) show the excitonic effect on the optical response in (8,0) and (10,0) carbon nanotube chain system. Graph (3) (a) shows the (8,0) carbon nanotube chain system, the exciton binding energies for the first and second peak of the carbon nanotube were found 0.46 and 0.47 ev. The obtained values were less than previously obtained results. This difference was due to different screening used in calculations. Graph (3) (b) shows the results of (10,0) carbon nanotube chain system. The binding energies of the two direct carbon nanotube excitons were 0.35 and 0.49 ev and the binding energy of the lowest (10,0) carbon nanotube exciton was found around 0.4 ev. In the case of the chain exciton, the binding energy was 0.38 ev. This value was close to the value of 0.42 ev in (8,0) carbon nanotube chain and the small difference was because of different values. The binding energy of direct excitons formed from the hybridized bands was 0.31 ev and indirect excitons was 0.18 ev which was slightly less than the (8,0) carbon nanotube chain system. The dashed curve in Graph (3) shows the total

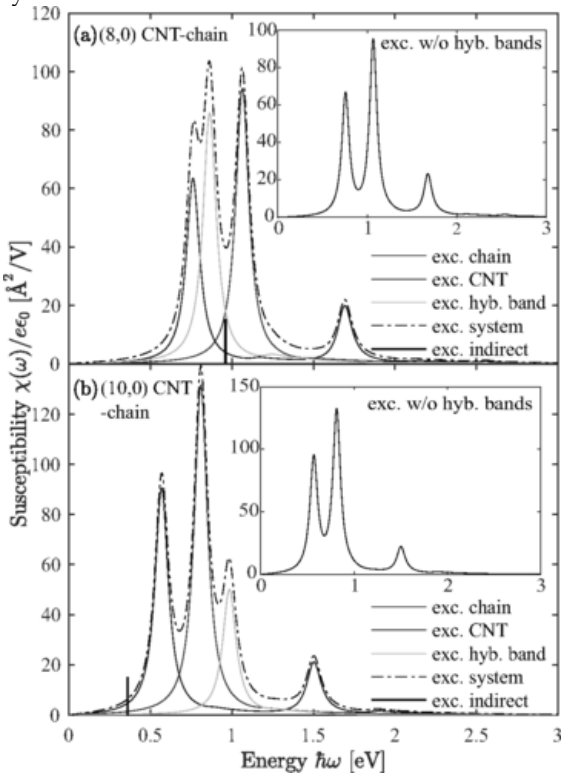
excitonic optical response of the system for energies close to the band gap for both systems. Indirect excitons were optically inactive i.e dark. Initial excitation were found bright state and relaxed to dark state through charge transfer. The separation of charge transfer between carbon nanotube and chain was found slow and was suppressed by faster electron-hole recombination processes. In the case of a (10,0) carbon nanotube chain system a very small probability of trapping electrons in dark sate because energy was lowest energy state of the system. The found results were compared with previously obtained results of theoretical and experimental research works and were found in good agreement.



Graph 1: Plot of band structure of (8,0) carbon nanotube chain system vs without band hybridization.



Graph 2: Plot of single electron linear susceptibility for (8,0) carbon nanotube chain system vs carbon nanotube chain system with hybridization.



Graph 3: Plot of Bethe-Salpeter sult for the excitonic linear susceptibility of (8,0) carbon chain system vs (10,0) carbon nanotube chain system with and without hybridization.

CONCLUSION

The study of optical response of single electron and excitonic systems in carbon nanotubes were made. We have calculated the band structure of the system applying density functional theory approach and compared with calculated results of band structure applying tight binding approach. The tight binding band structure allowed for the computation of the optical response. The band structure of the system changed by means of interactions between subsystems and a new band gap and optical transitions in combined system. It was found that these interactions affected the electronic structure of the system and produced indirect band gap. The changes in electronic structure demonstrated the changes in the single electron and also excitonic optical response of the system by new optical transitions. The obtained results presented that electron and holes were on the isolated carbon nanotube and chain. The obtained results were found in good agreement with previously obtained results.

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