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Strain Dependent Electronic Structure and Optical Response of Carbon Nanotube

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ABSTRACT One dimensional quasi-particles for low dimensional systems there is less surrounding material than in bulk systems, leading to weak dielectric screening of the electron-electron and electron-hole interaction. As a consequence quasi particle shifts are as large and excitonic effects were found strong. In order to produce strain sensing based on carbon nanotubes electronic and optical properties as well as strain dependence, so it is essential for the development of micro opto-electro mechanical systems, such as strain tunable emitters based on carbon nanotubes or tunable optical sensors. We have used first principles for electronic structure calculations based on G. W. approximation and Bethe-Salpeter equation to obtain strong strain related shifts in the optical absorption spectrum of carbon nanotube. We have found that exciton binding energy in strained carbon nanotubes is a function of the band gap and study leaded to strain dependent inhomogeneous dielectric screening. This presented that deformation potentials of electronic eigen-values and exciton binding energies were considered for the solution of strain dependent optical spectra of carbon nanotubes. The scaling relation allowed to extrapolate the shift of optical transition from the unstrained to the strained state based on the strain induced shift of electronic energy levels.

KEYWORDS Quasi-particles, Dielectric Screening, Excitonic Effect, Exciton, Strain, Deformation Potential, Optical Transition.

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INTRODUCTION

Spataru and Leonard [1] presented quantitative picture of the strain behavior of optical transitions because their dependence on the single particle band gap of the carbon nanotube was not straight forward. This was attributed to strong manybody effects. In the case of low dimensional systems such as quasi one dimensional carbon nanotubes have less surrounding material than in bulk systems [2]. In carbon nanotubes the mechanical behavior dominated by high stiffness and large rapture strain [3-4] and are chemically very stable [5] and showed a sizable shift of electronic energy levels as a function of axial strain [6-8]. The shift rendered optical transitions sensitive to strain has been observed and explained theoretically and experimentally [9-11]. The optical strain sensors with extremely high, mechanically

tunable sensitivity was built in combined carbon nanotube and micro-electro mechanical systems [12-14]. The spatially resolved dielectric function $\in\left(r,r'\right)$ was needed to the actual electron density of the carbon nanotube [15] and was found strongly direction dependent. In many studies only the dielectric constant $\in$ was used as screening model for the description of excitons in carbon nanotubes because it is a much simpler quantitiy [16-18]. Hohenberg et al. [19] and Kohn et al. [20]used to compute ground state geometries and total energies of a small diameter carbon nanotube in equilibrium and under axial strain. Huser et al. [21] and Qiu et al. [22] studied the slow decay of the coulomb interaction with distance rendered to eliminate artificial interaction between periodic images. Shim et al. [23] developed on analytical framework to derive upper bounds light matter interaction in the optical near field where applications from spontaneous emission amplification to greater than block body heat transfer showed transformative potential, these limits demonstrated the possibility of orders of magnitude enhancement in near field optical response with the right combination of material and geometry. St. Gelais et al. [24] and Song et al. [25] studied that Raman scattering and greater than block body transfer of thermal energy. All previous bounds and sum rules [26-28] the material figure of merit derived general quantitative. In a frequency bandwidth phase space was mapped out which materials were optimized. Taniguchi [29] studied theoretically the control and enhancement of linear and nonlinear thermo-electricity by regulating quantum coherence in nanostructure such as quantum dot. It was found that in nanostructures, the typical temperature scale was much smaller than the resonance width largely suppressed thermoelectric effects. Chen et al. [30] studied correlated optical state involved in controlled interactions between individual single photons through linear and nonlinear medium then a more efficient was used the evolution of multi photons in the highly optical medium. This approach mimics the dynamics of manybody systems with adjustable interactions strength allowed to simulate state transfer on a spin chain by tuning the interaction. Flamini et al. [31] presented that the photonic system was widely regarded as an ideal platform for quantum computation and quantum computation to its long coherent time and accurate single qubit operation. Krastanov et al. [32] studied the universal quantum computation was realized through the linear and nonlinear optics in the quantum region. Advances in materials and technologies[33-36] offered promising avenues for the quantum regime of linear and non-linear optics. The simulators was made based on solid state system such as ion traps and ultra-cold atoms.

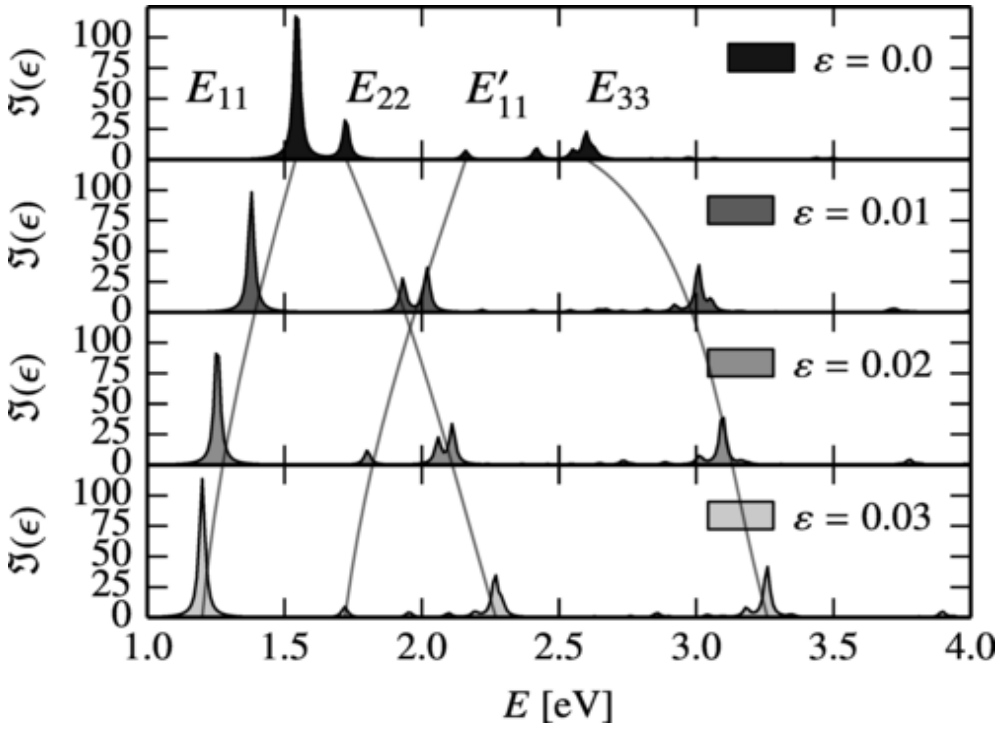
METHOD

We have used first principles electronic structure calculations for the study of our problem. We have considered density functional theory to compute ground state geometries and total energies of a small diameter carbon nanotube in equilibrium and under axial strain. G. W. approximation was used to account for quasi-particle effects on electronic energy levels. We have derived strain induced shifts of valence and conduction band energies and compared to results from a computationally cheaper hybrid exchange correlation functional. By solving Bethe-Salpeter equation for the optical polarization function we have accounted for excitonic effects in optical absorption spectra. We have studied the influence of coulomb truncation a scheme used to mitigate finite size effects in supercell calculations for low dimensional systems and optical spectra of carbon nanotube under axial strain was produced. These calculations of optical transitions allowed disentangling the influence of strain on quasi-particle energies and on excitonic effects. The relation between exciton binding energy reduced effective mass and dielectric constant. The local density approximation was used to describe exchange and correlation and the electron-ion interaction was described using norm-conserving pseudopotential based on the parameterization by Von Barth and Car. Wave functions were expanded into a plane wave basis upto a cutoff energy. We have compared the calculated results within the Vienna ab initio simulation package. We have used the generalized-gradient approximation of Perdew, Burke and Ernzerhof and the projector augmented wave method. The

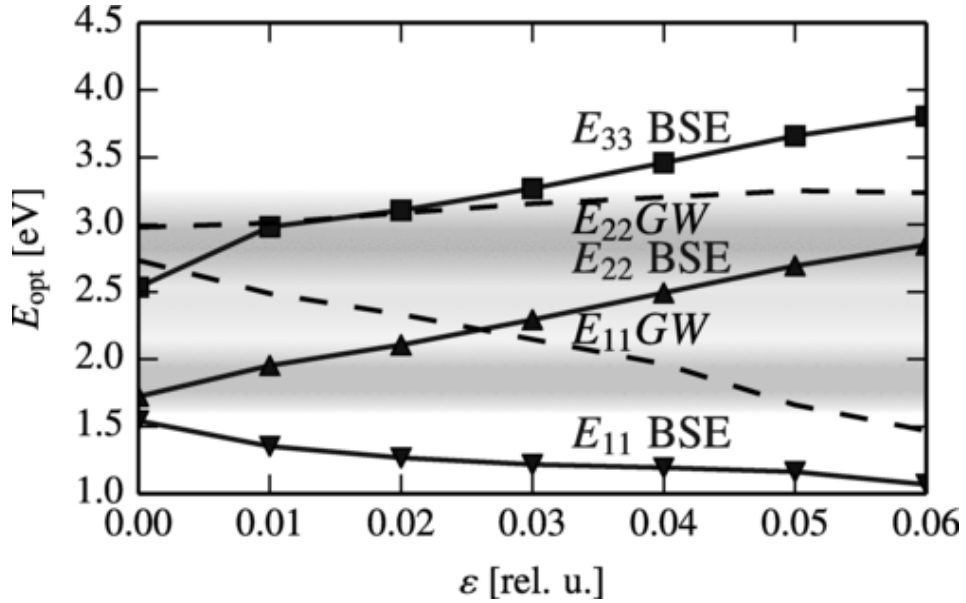
calculations were made using a plane wave cutoff energy of 400 ev and the same k-point grid. The resulting strain dependencies of exciton binding energies and optical transitions were essential ingredients for design and layout of micro opto electron mechanical systems. To compute total energies via minimization of Hellman-Feynman forces, optimized ground state geometries of a (8,0) carbon nanotube in equilibrium as well as under axial strain. The obtained results were found in good agreement with previously obtained results.

RESULTS AND DISCUSSION

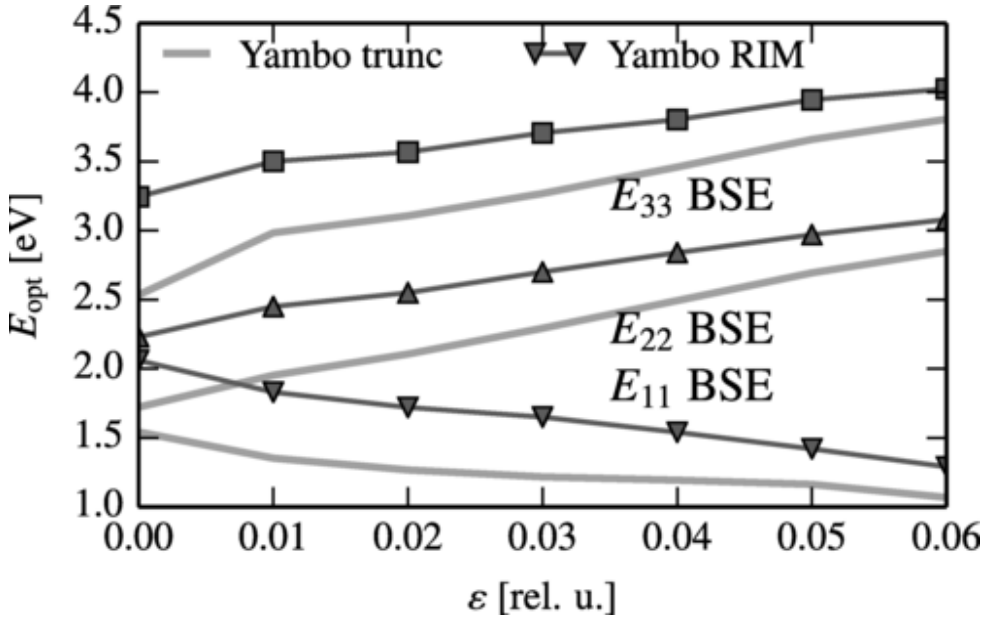
Graph (1) shows the plot of strain dependent optical spectra of the (8,0) carbon nanotube. This indicates the spectra is strain induced shift of the transitions. The unprimed transitions denote first order excitations, whereas the primed transition is a second order exciton that originated from the same electronic bands. This relied on the numerical diagonalization of the exciton Hamiltonian, whose eigen-states are super positions of non-interacting KS states. These contributions were analysed for the different strained cases. Graph (2) shows the plot of optical transition energies for the strained carbon nanotubes with excitonic effects. The visualization of strain depended optical transitions is also seen, the first and 2nd optical transition shift in opposite direction under strain are present. This is consistent with the most simple tight binding calculation of the carbon nanotube electronic bands with the zone folding method applied which predicted a down shift of carbon nanotube bands with strain for odd transitions and up shifts of even carbon nanotube. Graph (3) shows the plot of optical transitions appeared at lower energies when the coulomb interaction is truncated, which means that corresponding exciton binding energies are larger. The untruncated case hold the electron hole interaction and affected by periodic images over long distances but in the truncated case no periodic images are present and only the much smaller vacuum screening contributions are present. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.



Graph 1: Plot of strain depended optical spectra of the (8,0) carbon nanotube.



Graph 2: Plot of optical transition energies for the strained carbon nanotube with excitonic effects.



Graph 3: Plot of optical transitions for lower energies.

CONCLUSION

We have studied the strain dependent electronic structure and optical response of carbon nanotube. For electronic and optical strain sensing and optical strain characterization, which is promising technique due to practical ease of optical readout and higher precision compared to alternative approaches such as indirect electronic characterization. The optical strain sensors with extremely high mechanically tunable sensitivity are built in combined carbon nanotube and micro opto electromechanical systems. We have found that exciton binding energy in strained carbon nanotubes is a

function of the band gap and work leaded to the conclusion that this arised directly from strain dependent inhomogeneous dielectric screening. This indicates that deformation potentials of electronic eigen-value and exciton binding energies needed to be considered for the prediction of results. We have found that large deformations were possible in carbon nanotubes before rapture, which allowed exploring a much larger strain than in bulk materials. The obtained results were found in good agreement with previously obtained results.

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