

Electronic Structure of Chiral Collapsed Carbon Nanotubes and Characteristics of Flat Bands

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ABSTRACT	The study of characteristics of different sizes of flat bands were made. The study of chiral nanotubes were made and was found that the threshold diameter of free standing carbon nanotubes were of collapsed nature and were dependent on chirality and interlayer registry. In this process the symmetric breaking was also considered due to collapse. The registry was improved by interlayer shear. The study of electronic structure of collapsed cases were made and small band gap was found by means of confinement in flat band due to curved edges. But in the case of zigzag carbon nanotubes three small gap in semiconductor was produced and was dependent on width and band gaps. A monotonic feature gave rise to magic angle.
KEYWORDS	Electronic structure, chiral collapse, flatband, symmetric breaking, confinement, chirality magic angle.

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INTRODUCTION

Zhang et al. studied that carbon nanotubes of collapsed features and were found having high member of atoms and free standing collapsed carbon nanotubes and was found to have higher threshold [1]. Sanchez and Espino studied the transport phenomena at twist angle [2]. Chen et al. studied chiral phonons due to absorbing atoms on graphene and were found quantized at higher symmetry points. The phonon chirality induced absorption was found of non-phonon Berry curvature. The non-equilibrium phonon

distribution produced angular momentum and Hall current in absorbed grapheme [3]. Tang et al. studied that carbon nanotubes were found stable upon collapse with sizeable at small chiral angles consisting of higher number of atoms in cells [4]. Barzergar et al. studied the role of chiral collapsed carbon nanotubes for twisting deformations of collapsed carbon nanotubes and found a potential relation with magic angles [5]. Ueda et al. and He et al. experimentally observed the existence of chiral phonons having non zero polarization in hexagonal lattice having broken spatial inversion symmetry and it

was found that chiral phonons have role in electron valley scattering [6,7]. Xiong et al. studied the creation of effective magnetic field and coupling of electrons [8]. Chen et al. studied the phonon polarization in x and y directions of total angular momentum of nonmagnetic system and was found zero due to odd function distribution having time reversal [9]. Liu et al. studied stability and electronic structure of different tubes using density functional theory [10]. Cole and Andrews studied the optical chirality density in free space for a monochromatic beam and it was found that optical chirality was independent of orbital angular momentum [11]. He et al. studied the stability upon collapse having sizeable small chiral angles for different diameters and produced large number of atoms. The deposition on a substrate became less and it was found related to symmetry operations [12].

METHOD

Simulation of collapsed carbon nanotubes was made by means of molecular dynamics calculations. This explained the structure and flat bands creation. This created corrugation in flattered bilayer of carbon nanotubes. The band was found considering tight binding model. For this purpose the following expression was used.

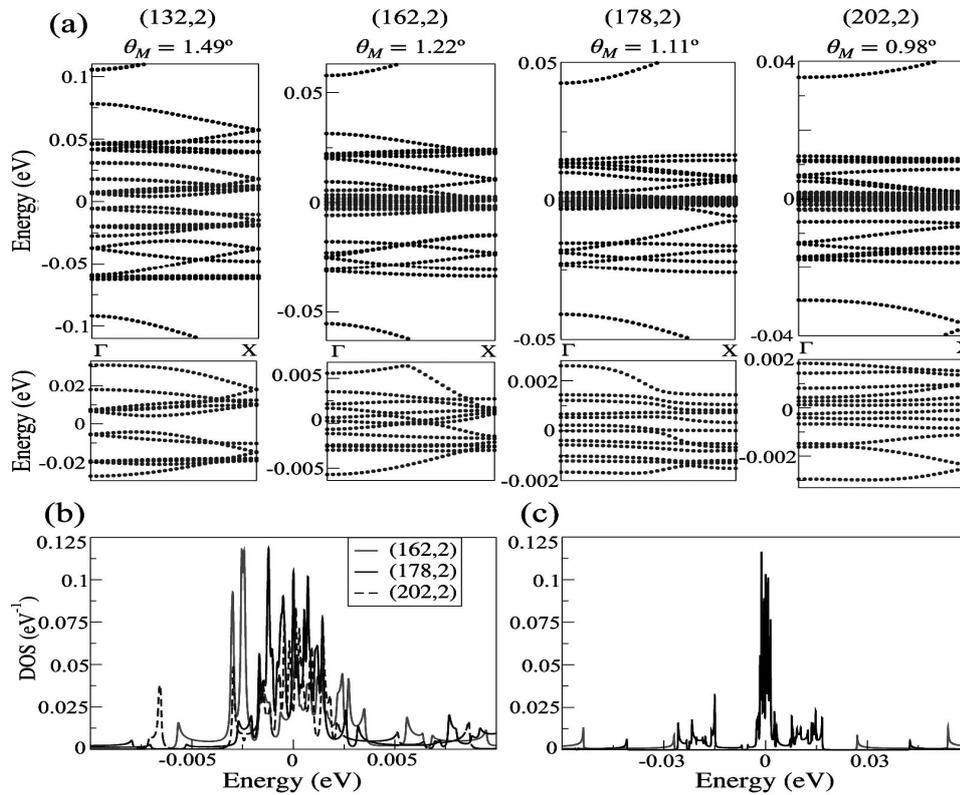
$$H = -\sum t(R_i - R_j) |R_i\rangle \langle R_j| + H.c.$$

Where $|R_j\rangle$ is the wave function and (R_i) is the position of atom. The molecular dynamics calculations presented flattered central region and moires were found. The density functional theory was considered for conducting carbon nanotubes by using SIESTA code having parameter containing Brillouin zone. A model of twelve unit of cell was considered for simulation for different atoms. The Hexagonal

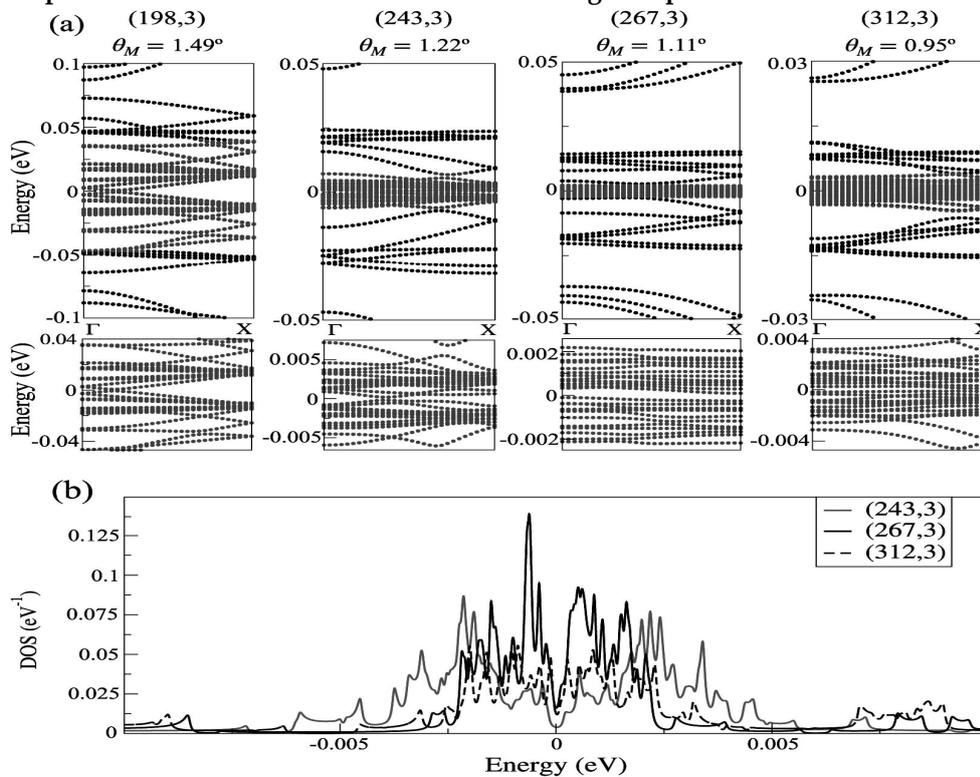
orthorhombic unit cells were used for the study of carbon nanotubes collapsed cases. The Brillouin zone sampling was used having dense k -point meshes for armchair and zigzag collapsed carbon nanotubes.

RESULTS AND DISCUSSION

The stacking in collapsed carbon nanotubes of armchair and zigzag edges were studied and it was seen shearing for generation of central zones in staking and translational intermediates. In the case of bilayer graphene behaved as turbostratic stacked like decoupled materials but stronger coupling in band structure was found. It produced collapsed tubes having intermediate interplay stacking. In the case of different diameters armchair carbon nanotubes, the energy difference between flattered and cylindrical tubes were used to obtain threshold diameter but the collapsed tubes were found stable. Graph (1) (a) shows the flattering and isolation of the central bands of several carbon nanotubes and it was found that moire angle decreased. It was seen that different optical and electronic properties were responsible for increase of differences of moire. It was found that the classification did not affect the flattering of the central bands of the carbon nanotubes. The larger probability of strongly correlated electronic behaviour was found. Graph (1) (b) shows the density of state for largest semiconducting carbon nanotubes. Graph (1) (c) shows the effect any of collapse on the density of state for spans of the bands of carbon nanotubes in the case of cylindrical and collapsed tubes. It was found that space created peaks which showed high localization of these states. Graph (2) (a) shows the Dirac crossing of carbon nanotubes. It was presented in the leftmost panel. The isolated and flattered having inner set were found very flat band. Graph (2) (b) shows the density of state of tubes.



Graph 1: Plot of band structure of semiconducting collapsed carbon nanotubes.



Graph 2: Plot of density of states of largest carbon nanotubes.

CONCLUSION

The study of structure of chiral carbon tubes and characteristics features of flat bands were made. The chiral carbon nanotubes collapsed cases were made by molecular dynamics. It was found that the geometry and moiré dissipation of characteristic of flat bands were available. The carbon nanotubes showed similar to that of magic angles tuning as monotonic nature and produced magic angles for twisted bilayer carbon nanotubes and graphene. The magic angle nature of carbon created moiré potentials. The results showed that moiré patterns which was universal, when chiral angle was small having localized states collapsed was dependent on, in response to threshold diameter having chirality and interlayer registry.

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