行政院國家科學委員會專題研究計畫 成果報告

石墨相關系統與二維調變電子系統的物理特性

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The main results are as follows:

(I) **Optical Spectra of AB- and AA-Stacked Nanographite Ribbons**  
by C. W. Chiu, F. L. Shyu, C. P. Chang, R. B. Chen, and M. F. Lin  
(J. Phys. Soc. Jpn. 72, 170-177(2003))

Abstract:

The absorption spectra of the AB- and AA-stacked nanographite ribbons have several prominent peaks. They strongly depend on the edge structure, the ribbon width, the stacking sequence, and the polarization direction. The armchair ribbons quite differ from the zigzag ribbons. The frequency and the number of the absorption peaks are affected by the ribbon width. The AB-stacked systems have lower threshold absorption frequency, more absorption peaks, and weaker spectral intensity, as compared with the AA-stacked systems. The absorption spectra are highly anisotropic. The optical excitations of the parallel polarization (E∥z) are absent in the AA-stacked systems. Comparison with graphite is discussed.

(II) **Uniaxial-Stress Effects on Electronic Structures of Nanographite Ribbons**  
by C. P. Chang, Y. H. Chen, F. L. Shyu, R. B. Chen, and M. F. Lin  
(Physica E, 18, 509-522(2003))

Abstract:

The uniaxial-stress effects on the low-energy electronic properties of nanographite ribbons are studied by the tight-binding model. The dependence on the strain, the edge structure, the ribbon width, and the stacking sequence is strong. The strain could induce the alternation of energy dispersions, the destruction of state degeneracy, the variation of energy gap, the semiconductor-metal transition, and the change of special structures in density of states. The effects of strain are important for the AB- and AA-stacked armchair ribbons. However, they are negligible for the AB- and AA-stacked zigzag ribbons. Armchair ribbons could exhibit the semiconductor-metal transition. Such transition is mainly determined by the strain and the ribbon-ribbon interactions.
Abstract:

The low-frequency magnetoplasmons of armchair carbon nanotubes are investigated by the random phase approximation. The dependence on the magnetic flux $\psi$, the direction $\alpha$ of magnetic field, and the temperature $T$ is novel. Each nanotube exhibits one interband magnetoplasmon at low temperature, when the magnetic field is not perpendicular to the nanotube axis. The plasmon frequency decreases (increases) with $\alpha$ ($\psi$), while the strength of plasmon exhibits the opposite behavior. One interband and intraband magnetoplasmon can exist at $\alpha = 90^\circ$, and it is almost the same with that in the absence of $\psi$. The temperature can induce one intraband magnetoplasmon and reduce the frequency of the interband magnetoplasmon. The new plasmon is absent at low $T$, or at high $T$ and large $\alpha$. The $T$-dependence is negligible for the interband and intraband magnetoplasmon at $\alpha = 90^\circ$ or the plasmon at $\psi = 0$.

Abstract:

The low-frequency single-particle and collective excitations of the single-walled carbon nanotubes are studied in the presence of magnetic field. They strongly depend on the magnitude and the direction of magnetic field, the transferred momentum, the temperature, the nanotube geometry, and the Zeeman splitting. A narrow-gap nonarmchair carbon nanotube exhibits two interband magnetoplasmons, while a metallic nonarmchair carbon nanotube exhibits one interband magnetoplasmon and one interband and intraband magnetoplasmon, or two interband magnetoplasmons and one intraband magnetoplasmon. The differences among these plasmons are relatively obvious, when the magnetic field is oriented closer to the nanotube axis. The transferred momentum determines the plasmon frequency and the existence
of plasmons. The temperature can induce a intraband magnetoplasmon, or change a interband magnetoplasmon into a intraband and interband magnetoplasmon.

(V) Magneto Electronic and Optical Properties of Carbon Nanotubes
by F. L. Shyu, C. P. Chang, R. B. Chen, C. W. Chiu, and M. F. Lin
(Physical Review B, 67, 045405(9)(2003))

Abstract:

Magnetoelectronic and optical properties of carbon nanotubes are, respectively, studied within the $sp^3$ tight-binding model and the gradient approximation. They strongly depend on the magnitude and the direction of the magnetic field, the nanotube geometry (radius and chiral angle), and the Zeeman splitting. The magnetic field would lead to the change of energy gap, the destruction of state degeneracy, and the coupling of different angular momenta. Hence there are magnetic-field-dependent absorption frequencies and more absorption peaks. The types of carbon nanotubes predominate in the band structure and thus the range of absorption frequencies and the number of absorption peaks. The Zeeman splitting makes the semiconductor–metal transition occur at lower magnetic flux. It metalizes armchair carbon nanotubes in the presence of the perpendicular magnetic field. However, it does not affect the optical excitations except for metallic carbon nanotubes.

(VI) Magneto Energy Gap of a Single-Walled Carbon Nanotube
by F. L. Shyu, C. P. Chang, R. B. Chen, and M. F. Lin

Abstract:

Magnetoelectric energy gap of a single-walled carbon nanotube is calculated by the $sp^3$ tight-binding model. It strongly depends on the direction and the magnitude of the magnetic field. There is no simple relation between the energy gap and the magnetic field. This result quite differs from the previous predictions.