Programs & Abstracts

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P.28 – Poster, NCTP-40

EFFECT OF TEMPERATURE ON ELECTRON EFFECTIVE MASS AND BAND-GAP IN SEMICONDUCTOR CARBON NANOTUBES

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The effect of temperature on the self-energy of electron in semiconductor carbon nanotubes are studied by Matsubara Green function approach. Numerical results show a large influence of the temperature and electron density on the band-gap and electron effective mass in semiconducor carbon nanotube

Presenter: Tan Van Le

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Surface optical phonon-assisted cyclotron resonance in graphene on a h-BN substrate

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In this work, the influence of surface optical (SO) phonons on the phonon-assisted cyclotron resonance (PACR) effect has been theoretically studied in a single-layer graphene on h-BN substrates via both one and two-photon absorption processes. The two-photon absorption process gives a significant contribution to magneto-optical absorption coefficient (MOAC) compared to one-photon process. The shifts of the absorption peaks are larger for h-BN substrate than those in graphene on nonpolar substrates, where only the intrinsic optical phonons of graphene contribute. Effects of temperature, graphene-substrate separation, and magnetic field on the MOAC and the half width are discussed. Our results show that the h-BN substrate strongly influence on the magneto-optical absorption spectra not only in the magnitude but also in the position of the resonant peaks due to electron-SO phonon scattering.

Presenter: Huynh Vinh Phuc

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Temperature dependence of electron-hole pair condensation driven by exciton-phonon interaction

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A stability of the electron-hole pair condensation at low temperature has been addressed by involving the coupling of exciton to vibrational degrees of freedom in two-dimensional two-band $f - c$ electron system. By mean of the unrestricted Hartree-Fock approximation, we find a formation of the insulating state typifying an excitonic condensate accompanied by a finite lattice distortion if the exciton-phonon coupling is large enough. As functions of temperature

both excitonic condensation order parameter and lattice distortion behave in a same way which manifests the continuous transition in analogy to the superconductivity in the BCS theory. Inspecting to the microscopic properties in momentum space we strongly specify the BCS type of the excitonic condensation driven by the exciton-phonon interaction at low temperature.

Presenter: Do Thi Hong Hai

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Effects of pairing reentrance on the inverse nuclear level density parameter of hot rotating nuclei

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Angular momentum dependence of the inverse level density parameter K in the excitation-energy region of about 30 – 40 MeV is studied within the finite-temperature Bardeen-Cooper-Schrieffer (FTBCS) theory that takes into account the noncollective rotation of the nucleus at nonzero values of z-projection M of the total angular momentum. The comparison between the results obtained within the FTBCS as well as the case without pairing correlations and the experimental data for several medium-mass nuclei such as ^{108}Cd, ^{109}In, ^{112}Sn, ^{113}Sb, ^{122}Te, ^{123}I, ^{127}Cs, shows that by including the pairing corrections the FTBCS reproduces quite well all experimental data, whereas the non-pairing case overestimates the data. As the result, within the FTBCS, there appears an effect that pairing correlations is first small at a given value of angular momentum M, which is close to its critical value MC, where pairing is completely disappeared, and zero temperature ($T = 0$), increases with increasing T, and then decreases to vanish at high T. This effect is called the pairing reentrance.

Presenter: Le Thi Quynh Huong

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Surface Properties of TiO2 from Self-Consistent-Charge Density Functional Tight Binding

Huynh Anh Huy (1), Vien Tuan Anh (1), Nguyen Vy Khuong (1), Le Thi Cam Loan (2)

(1) Can Tho University, (2) Tra Vinh University

Anatase and rutile TiO2 surfaces have been investigated with a computationally efficient semiempirical tight binding method: self-consistent-charge density functional tight binding (SCC-DFTB). SCC-DFTB predicts a band gap of anatase TiO2 surface of 2.3 eV comparing with one of rutile TiO2 surface of 1.9 eV. The OH group has been found when hydrogen adsorbed on the anatase (001) surface and water molecules on rutile (110) surface.

Presenter: Viên Tuấn Anh

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Dynamics Simulation of Backward Diffusion Based on Random Walk Theory

Vu Ba Dung and Bui Huu Nguyen