The Asian Network School and Workshop on Complex Condensed Matter Systems 2018

Report of Contributions

https://indico.cern.ch/e/ICTPANSSUT

Contribution ID: **7** Type: **not specified**

Photoemission studies of complex condensed systems

Track Classification: School

Contribution ID: **8** Type: **not specified**

Atomic Arrangement and Its Effects on Electronic Structures of Graphene from Tight-Binding Description

The electronic structures of pristine graphene can be qualitatively described by tight-binding method. Tight-binding model is a simple method to understand the contributions of each atomic state. The method is helpful to investigate how chemical bonding, atomic arrangement, and structural symmetry reflect to the electronic structure of a system. Structural stability of monolayer graphene with dopants or impurities is able to be systematically investigated by means of first-principles calculations. However, the method is more expensive than simple tight-binding approximation. Tight-binding method provides an insightful of how the interactions between the constituents influence on the characteristic of electronic structure, which is sensitive to the detailed arrangement of the constituents. Tight-binding calculations of several representative ordering patterns including ribbon, superlattice (SL) or stripe, and scattering arrangements are given to illustrate an idea of how to construct Hamiltonian matrix for such systems. These matrix elements are considered as parameters, which are fitted to reproduce certain properties from experimental data or first-principles calculations. The properties of nanoribbons and superlattices along armchair and zigzag direction have been discussed in the context of the tight-binding approximation, as they provide an informative trend of the electronic properties related to edge modification and inversion symmetry of structure.

Ref http://110.170.84.132/ccmp/sirichok/doc/graphene.pdf

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Presenter: Dr JUNGTHAWAN, Sirichok (School of Physics, Suranaree University of Technology)

Track Classification: School

Contribution ID: **9** Type: **not specified**

First-Principles Electronic Structure Calculations of MgZn-based Ternaries

The present talk will discuss the computed results of electronic energy band structure, partial density states, total density of states and electronic charge density for nine MgZn-based metallic complexes: MgZnCo2, MgZnRh2, MgZnIr2, MgZnNi2, MgZnPd2, MgZnPt2, MgZnCu2, MgZnAg2, and MgZnAu2. The first principles electronic structure calculations is made by employing density functional theory as implemented in Quantum Espresso. All the nine materials belong to the cubic class of Bravais Lattice with space group Fm m (in full detail it is F 4/m 2/m) and space group number 225. The Pearson symbol for them is cF16, i.e. it is a face centred cubic system consisting of 16 atoms for complete representation of conventional unit cell. All the ternaries are found metallic by nature. The band structure is found more dispersive along the path K-Γ-L. An indirect band separation below the Fermi level is seen at around 6.23, 6.08, 6.21, 5.37, 6.27, and 6.48 eV for MgZnNi2, MgZnPd2, MgZnPt2, MgZnCu2, MgZnAg2, and MgZnAu2. The highest peak in DOS is due to d-orbitals of Zn and it is located around 7 eV below the Fermi level. The Charge density plots show that highest electron density is around Zn and lowest around Mg. The charge density between Zn and the substituted atom (Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, and Au) is more compared to other interactions. It is also found that MgZnCu2 has 100 times more charge density at the minimum scale compared to the other eight ternaries.

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Contribution ID: **10** Type: **not specified**

Vibrational effects to unidirectional π-electron rotation in an aromatic ring molecule with low-symmetry

Recently we proposed a new lasers-control scheme for unidirectional π-electron rotation in an aromatic ring molecule with low-symmetry having no degenerate electronic states [1]. In this control scheme we assumed a fixed nuclei condition, and two relevant excited states subject to dynamical Stark shift using two linearly polarized UV lasers. Each laser is set to selectively interact with one of the two electronic states, the lower and higher excited states are shifted up and down with the same detuning, respectively, and two excited states become degenerate at their midpoint.
In this presentation for more realistic numerical simulation of unidirectional pi-electron rotation, we take into account the nuclear vibrational effect in a molecular system. The total wave function is separated into electronic and nuclear parts under the B.O approximation. The vibrational states in each excited state follow the Franck-Condon principle. It is also interesting to investigate the interactions between the relevant two electronic states through the vibronic (non-adiabatic) couplings, and the vibronic couplings through the breakdown of the B.O approximation can be estimated at the equilibrium nuclear distance. We show a result of numerical simulation and discuss how the nuclear vibrations affect the unidirectional pi-electron rotation.
Reference
[1] H. Mineo, M. Yamaki, G.S. Kim, Y. Teranishi, and Y. Fujimura, Phys. Chem. Chem. Phys. 18, 26786 (2016).

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Contribution ID: **11** Type: **not specified**

Electronic and transport features of sawtooth penta-graphene nanoribbons via substitutional doping

In this work, electronic and transport properties of a pristine sawtooth penta-graphene nanoribbon (SSPGNR) and sawtooth penta-graphene nanoribbons doping with Silic, Nitrogen, Phosphor (Si-SSPGNR, N-SSPGNR, P-SSPGNR) are studied systematically by density-functional theory in combination with the non-equilibrium Green's function formalism. Pristine sample and three doped samples in a similar position are terminated with H atoms. To explore in detaided the electronic and electron transport features, we compute and discuss about the structure properties, bandstructure, density of states, I-V curve, device density of states and tranmission spectrum. Our result shows that doping affects dramatically on the electronic nature and the I-V characteristic of samples. More specifically, the intensity of current of N-SSPGNR and P-SSPGNR increase by 8 orders of magnitude compared to SSPGNR while the one of N-SSPGNR change negligible. However, there are also considerable differences in I-V curves of samples doping with N and P. Our findings indicate that the doping by N, P can effectively modulate the electronic and transport properties of SSPGNRs which has not been studied so far.

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Contribution ID: **12** Type: **not specified**

Electronic transport properties of sawtooth penta-graphene nanoribbons under edge passivation by non-metallic atoms

The transport properties of sawtooth penta-graphene nanoribbons (SS-PGNRs) are investigated using density functional theory in combination with nonequilibrium Green function. The configurations are theoretically studied in terms of a bare edge and edges terminated by non-metallic atoms (H, P, Si) such as : symmetrical edge terminations (HH-SS-PGNR, PP-SS-PGNR and SiSi-SS-PGNR) and alternate edge terminations (PH-SS-PGNR and SiH-SS-PGNR). It is found that SS-PGNR band gap can be controlled through changing various edge termination, which leads to the transition from a semiconductor to a half-metal or to a metal. In effect on transport properties, P and Si atoms improve significantly the current intensity in alternate cases. The obvious reduction of current is observed in HH-SS-PGNR and PP-SS-PGNR. Interestingly, oscillation current-voltage characteristic appears when PGNR is passivated symmetrically by Si atoms. These outcomes derive from the strong dependence of SS-PGNRs on type of terminated atom at the edge of ribbon and could be used to design novel nano-electronic devices.

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Contribution ID: **13** Type: **not specified**

Emergent holographic description for the Kondo effect: Comparison with Bethe ansatz

We propose one concrete realization of the holographic duality conjecture, implementing Wilsonian renormalization group transformations in a recursive way.
In other words, starting from an effective ultraviolet (UV) boundary quantum theory,we derive its corresponding infrared (IR) bulk classical field theory,
which appears naturally in one-dimensional higher spacetime.

It turns out that the emergent extra dimension can be identified with an energy scale of the renormalization group transformation. We find that an effective bulk equation of motion encodes all-loop quantum corrections through the extra dimension,organized in the 1/N expansion, where N represents the flavor number of strongly correlated quantum fields.

We implement this recursive Wilsonian renormalization group method to the Kondo problem. The perturbation approach in the vicinity of the decoupled local moment fixed point breaks down, approaching the Kondo temperature, where only three theoretical frameworks can access this crossover regime,including the strong coupling IR fixed point until now: Wilson's numerical renormalization group method, Bethe ansatz,and conserving t-matrix approximation. As a result, we succeed in describing the crossover regime from a weakly correlated local moment fixed point at high temperature to a strongly coupled local Fermi-liquid fixed point at low temperature in a nonperturbative way, where the characteristic energy scale is given by the Kondo temperature.

Impurity thermodynamics in our non-perturbative description is qualitatively well matched with the Bethe ansatz for the Kondo effect.

Previously, we applied essentially the same technology into an emergent geometric description for a topological phase transition in the Kitaev superconductor model, which allows us to extract out an emergent metric structure [Ki-Seok Kim, Miok Park, Jaeyoon Cho, and Chanyong Park, Phys. Rev. D 96, 086015 (2017)].

Based on the Ryu-Takayanagi Formula with our derived metric tensor, we calculated holographic entanglement entropy. Interestingly, it turns out that this entanglement entropy reproduced the Cardy's formula perfectly not only at but also near the quantum critical point.

Primary author: Prof. KIM, Ki-Seok

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Contribution ID: **15** Type: **not specified**

Damping of spin waves in the spin polaron theory

The damping of spin waves in high-Tc cuprate superconductors was analytically calculated using the spin polaron formulation in the finite temperature Green's function scheme. This representation describes holes as spinless fermions and spins as normal bosons which are characterized by hard core bosonic operators obtained using the Holstein-Primakoff transformation. The interaction between the holes and spins are described by the spin polaron Hamiltonian which resembles the classic polaron interaction Hamiltonian. The expression for the attenuation of spin wave was obtained by calculating the second-order spin wave self-energy and taking its imaginary component where it involves taking the spectral function of the hole and spin wave Green's functions and a summation over the Matsubara frequencies. The rate of attenuation of spin waves was also obtained for a system with zero temperature and a low frequency limit.

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Track Classification: School

Contribution ID: **16** Type: **not specified**

Effect of error tolerance probability to the fidelity of a 4-qubit quantum search simulation

We simulate the optimized fixed-point quantum search (OFPQS) algorithm with first- and second-nearest neighbor interactions in a 4-qubit Ising spin system using a nonrefocusing technique. In order to perform a single qubit gate, we utilize the coupling interactions to control the neighboring spins. The phase-marking scheme of the OFPQS is implemented using a single rotation about the transverse axis instead of the usual rotation about the field axis. Furthermore, the state of the ancilla is initialized in a superposition of the basis states to avoid the generation of unwanted states. This procedure gives us a probability of finding the target state within the prescribed bound of the OFPQS. Based on this scheme, we investigate the effect of error tolerance probability of the OFPQS to the fidelity of the nonrefocusing implementation.

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Track Classification: School

Contribution ID: **17** Type: **not specified**

Detection and trace analysis of Rhodamine B using silver nanowires as surface-enhanced Raman spectroscopy substrates

The access to clean and potable water is an important challenge especially in Southeast Asian countries that are surrounded by bodies of water. Water contaminants such as dye effluents pose health hazards even in trace amounts and need to be accurately detected and quantified. Among various analytical techniques, Raman spectroscopy is recently becoming popular as a tool for the detection of pesticides, heavy metals, and organic dyes. In this work, we investigate the potential of silver nanowires (Ag NWs) as surface-enhanced Raman spectroscopy (SERS) substrates for the detection and quantification of organic dyes. The Ag NWs were synthesized through an electroless deposition method and stored in an alcohol-based colloidal suspension. The Ag NWs were deposited in a paper substrate that keeps the NWs from spreading. Rhodamine B (RhB) powders were diluted in varying concentrations and then dropped on the Ag NW SERS substrates. Micro-Raman spectroscopy was performed using a custom-built optical system under 532 nm optical excitation. The results showed that the Ag NWs SERS substrates can detect RhB up to a concentration of 1 μM. In addition, the SERS intensity follows a power law relation with the RhB concentration as shown by the linear fit in the log-log plot. The study demonstrates that SERS is a viable technique for the detection and quantification of trace contaminants in water with minimal preparation and using small sample amounts.

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Track Classification: School

Contribution ID: **18** Type: **not specified**

Entanglement entropy and area law in strongly-correlated systems

Understanding the nature of entanglement in strongly-correlated many-body systems is of prime importance in modern theoretical physics. In this lecture, I introduce the concept of entanglement entropies and the entanglement area law, and briefly review their implications in various topical issues. I then introduce a number of cases wherein the entanglement entropy can be analytically calculated, estimated, or bounded. In particular, I will discuss how the spectral gap, correlation functions, and the entanglement area law in strongly-correlated systems are mutually related to each other.

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Presenter: Prof. CHO, Jaeyoon (APCTP)

Track Classification: School

Contribution ID: **19** Type: **not specified**

Effects of varying tensile strain on the THz emission from epitaxially-lifted gallium arsenide quantum wells bonded onto flexible plastic substrates

Strain can change the physical and electrical properties of semiconductors. While strain can induce defects on semiconductors, its impacts are not always negative. Strain has been incorporated into semiconductor heterostructures to produce long wavelength (˜1.55 μm) gallium arsenide (GaAs) based lasers. The changes that strain can make on semiconductor electrical properties in particular allow for modulation of the band structure in GaAs-based bulk films and nanostructures such as quantum wells. This modulation in turn affects processes governed by photo-induced charges in the semiconductor crystal and may affect charge-reliant processes such as emission of Terahertz (THz) radiation.

In this work, the effect of varying tensile strain on the THz emission of AlGaAs/GaAs quantum wells is investigated. The quantum wells were grown using molecular beam epitaxy over an aluminum arsenide (AlAs) layer on a semi-insulating GaAs substrate. The AlAs was then etched away in diluted hydrofluoric acid to release the ˜1 μm thin film from its host substrate. The film was then bonded onto a flexible plastic sheet using surface tension forces. Photoluminescence spectroscopy was then performed on the bonded film as the plastic sheet was mechanically bent to induce varying levels of tensile strain. The PL shows that as the film is being bent, the band structure of the quantum wells effectively redshift by energies up to 13 meV relative to the unbent case. Reflection-mode THz time domain spectroscopy (TDS) was also performed while bending the sample and shows that the THz emission intensity from the sample is enhanced up to ˜20% relative to the unbent case. These results demonstrate that modulation of the band structure of GaAs quantum wells via strain can strengthen the THz emission from these heterostructures.

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Track Classification: School

Contribution ID: **20** Type: **not specified**

Uni- and bi-metallic small Pt and Ni clusters for fuel conversion applications: A DFT study

An ab initio density functional theory study was performed to investigate the adsorption of C and OH on small uni-metallic (Pt3 and Ni3) and bi-metallic (Pt2Re and Ni2Fe) clusters that could be potentially used for energy conversion applications. We observed that the HOMO-LUMO gaps show good stability and reactivity of the clusters. Furthermore, the introducing foreign atoms (Re and Fe) provides useful insights in designing and fine-tuning of these catalysts for energy conversion applications such as CO/CO2 methanation and hydrogenation reactions. Moreover, we observed that Pt3 and Pt2Re clusters bind with C and OH moderately, which could be utilized further for energy conversion.

Reference:
IOP Conf. Series: Journal of Physics: Conf. Series 1039 (2018) 012029

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Presenter: SANTOS-PUTUNGAN, Alexandra

Track Classification: School

Contribution ID: **21** Type: **not specified**

Electronic properties of TlFe2Se2 using density functional theory

Doping and anion height are found to drastically affect the electronic structures of superconductors [1-2]. In this study, we investigated the composition-dependence of the electronic properties of the newly discovered intercalated $TlFe_2Se_2$ superconductor using density functional theory. We calculated the electronic structures of $Tl_xFe_2Se_2$ with various Tl concentrations (x = 1.00, 0.75 and 0.50) using a 2 x 2 x 1 supercell. Fractional coordinate z_{Se} of Se which essentially controls the anion height are taken from "relaxed"nonmagnetic and magnetic configurations of $TlFe_2Se_2$ which have values of z_{Se} = 0.341 Å and 0.348 Å, respectively. We also used the experimental value of z_{Se} = 0.357 Å taken from [3], which is higher than the simulated ones. We also added a hypothetical value of z_{Se} = 0.364 Å which is the highest among the fractional coordinate values used. All calculations of the electronic structures are done using QUANTUM ESPRESSO [4]. Generalized gradient approximation of Perdew-Burke-Ernzerhof [5] is used for exchange-correlation potentials.

The density of states (DOS) for various Tl content has shown metallic properties where states near the Fermi energy (E_F) are mostly from Fe-d states. This is consistent with the typical features of iron-based superconductors. For various fractional coordinates, z_{Se}, the DOS have also shown similar characteristics. Band structure calculations on the other hand revealed different results. For x = 1.00, no pocket is found around the zone center (Γ point) of the First Brillouin zone. For x = 0.75 and 0.50 on the other hand, hole-like pockets are being observed around the Γ point which is typical of Fe-based superconductors. The appearance of the hole-like pockets might be due to the shifting of the E_F towards lower energy when Tl content is reduced. This indicates a possible doping effect in this material (i.e. hole doping).

Furthermore, we also studied the possible three dimensionality of $Tl_xFe_2Se_2$ with various Tl content by observing the Z point of the first Brillouin zone. As Tl content is reduced, a shift of bands is observed towards higher energies which resulted to an appearance of a shallow electron-like pocket around the Z point when x = 0.75. The electron-like pocket is mainly of Fe-d_{xz}+d_{yz} character. This is not consistent though with the experiments where the observed electron-like pocket has Fe-d_{xy}+Se-p_z character [6]. Looking at the band structure calculations for various z_{Se}, the electron-like band found around the Z-point above E_F for z_{Se} = 0.341 Å seems to shift towards lower energies as the z_{Se} increases, which eventually crossed the E_F for z_{Se} = 0.357 Å. This electron-like pocket is now consistent with the experimental results where the orbital character is found to be of Fe-d_{xy}+Se-p_z. Increasing further the z_{Se} to 0.364 Å, the bands split and a hole-like band is formed below E_F.

In conclusion, these results suggest that the Tl content plays a significant role in tuning the electronic properties of $Tl_xFe_2Se_2$ where doping effect might occur with the appropriate value of Tl concentration. In addition, the anion height shows strong control of the band topology of this material.

References

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Track Classification: School

Contribution ID: **22** Type: **not specified**

Settling behavior of YBa2Cu3O7−δ particles in Acetone in the presence of lead (IV) oxides particles

Electrophoretic deposition of YBa2Cu3O7−δ is a promising non-vacuum method of film deposition due to its simplicity and scalability. In order to produce high quality films using this technique, it is necessary for the working suspension to be stable for long periods of time. In this study, we look at the interaction of YBCO and PbO2 particles when suspended in acetone. We determine if PbO2 is a suitable compound that will allow stability in the YBCO-acetone suspension. The choice of PbO2 is based from our previous work where it was shown that PbO2 can be used as a flux during the partial melting step of the deposition process. The colloidal properties of YBCO and PbO2 in acetone were measured using hydrodynamic size and zeta potential measurements. Results show that YBCO particles are positively charged when mixed in acetone, while PbO2 particles were determined to be negatively charged. In addition, upon testing the suspension of YBCO+PbO2 in acetone, zeta potential measurements show a decrease in magnitude with respect to settling time. The addition of more PbO2 into the YBCO-acetone suspension also pushed its zeta potential values to the unstable region ($|\zeta| < 30$ mV). Due to this relatively strong Coulombic attraction of YBCO and PbO2 particles when mixed in acetone, electrophoretic deposition of YBCO with PbO2 will be difcult

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Track Classification: School

Contribution ID: **23** Type: **not specified**

Electronic properties of Monolayer FeSe on CaF_2 via DFT

A recent study on FeSe thin films grown on different substrates revealed that films on CaF_2 substrate has the maximum T_c ~15 K. However, the monolayer FeSe grown on $SrTiO_3$ (STO) substrate generated much research interest when superconductivity was observed at T_c above 100 K by means of *in situ* four-point probe electrical transport measurements. There are different factors that were identified, such as the tensile strain and electron doping, which contributed to the enhancement of the T_c. To investigate the interface effect in the superconductivity of monolayer FeSe, we calculated the structural and electronic properties of monolayer FeSe grown on CaF_2. Only electron pockets are observed around the M point for both NM and AFM configurations. The same feature is observed in experimental studies on 1ML FeSe/STO. This suggests that the mechanism of superconductivity of single-layer FeSe on STO and CaF_2 might be the same. However, further experimental research on 1ML FeSe/CaF_2 is necessary to verify our results.

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Track Classification: School

Contribution ID: **24** Type: **not specified**

Temperature-dependent conductivity of graphene in hybrid Bose-Fermi systems

We investigate finite temperature electron conductivity in a hybrid system consisting of spatially separated two-dimensional layers of graphene and condensed indirect exciton gas coupled via the Coulomb interaction. We calculate the energy dependent relaxation time of the electrons in the graphene layer accompanied by the emission and absorption of a single Bogoliubov excitation (bogolon). We further calculate the conductivity of graphene in this hybrid Bose-Fermi system. At last, we show, that bogolon-mediated scattering is predominant in hybrid systems, as compared with phonon-assisted relaxation.

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Track Classification: School

Contribution ID: **25** Type: **not specified**

Femtosecond pulsed laser deposition of BSCCO target on silicon substrate

We deposit films from a bulk Bi-2212 target via femtosecond pulsed laser deposition. Smooth as-deposited films with large substrate coverage were grown on Si (100). The annealed films reveal crystallization in more than one direction. The XRD spectrum confirms that the annealed film is polycrystalline with some peaks that may have come from dissociated BSCCO compounds. Further testing will be carried out for this preliminary study on the deposition of epitaxial high-temperature superconducting films.

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Track Classification: School

Contribution ID: **26** Type: **not specified**

Nonlinear Wave Spreading in Disordered Schrodinger Lattice

We study spatiotemporal evolution of wave packets of resolved normal density and energy density in a disordered discrete nonlinear Schrodinger chain. We prepare initial wave packets containing multiple-site excitations of given norm density and energy density in different regions of the equilibrium phase diagram of the discrete nonlinear Schrodinger chain. Multiple site excitations can evolve in the weak chaos or strong chaos regimes. We find an evidence of strong chaos in the discrete nonlinear Schrodinger chain. The total norm and total energy are conserved during the spreading of wave packets in time.

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Presenter: KATI, Yagmur

Track Classification: School

Contribution ID: **27** Type: **not specified**

Twisted bundle model for DNA toroidal condensates

We consider a model of DNA toroidal condensate that corresponds to a twisted bundle arrangement and compare it to other models of the chain conformation inside the condensate. The latter models correspond to those of a spool-like folding and a constant curvature bending. The ground states of the condensate in different models are obtained by minimizing a total energy given by the sum of the bending energy and a surface energy promoting compaction. It is shown that for the condensates of the same polymer length, the twisted bundle model leads to a lower ground state energy than both the spool model and the constant curvature model. A phase diagram of ground states depending on the chain length and the polymer stiffness is calculated for toroidal and rod-like condensates. We study also the curvature distribution and the thickness to radius ratio in optimal toroid condensates. Our study highlights the role of the twist geometry in DNA packing. The analytical results are supported by Monte Carlo simulations of a bead and spring model.

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Track Classification: School