From: "agaur" <agaur@iitk.ac.in>
Subject: [Scdt] PhD Oral exam of Ms. Juhi Srivastava (MSE), June 2nd @ 11:00 AM
Date: Mon, May 23, 2022 6:31 pm
To: acadstaff@lists.iitk.ac.in
Cc: dpgc_mse@iitk.ac.in,msepg@iitk.ac.in,msefc@lists.iitk.ac.in,"Deshmukh" <deshmukh@tifr.res.in>,"Saboo" <saboo@iitk.ac.in>,"Yogesh Chauhan" <chauhan@iitk.ac.in>,"Bsomnath" <bsomnath@iitk.ac.in>,scdt@lists.iitk.ac.in,jrkumar@iitk.ac.in,"Aniket" <aniket@iitk.ac.in>,govindb@iitk.ac.in

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Dear All,

Ms. Juhi Srivastava (Roll No. 14106264), a Ph.D. candidate in the Department of Materials Science and Engineering will defend her Ph.D. thesis titled "**Investigation of structural, vibrational, electronic and transport properties of Single-walled Carbon Nanotube - Single-layer Graphene hybrid nanostructures**" as per following details (in hybrid mode):

Date: June 2nd, 2022 (Thursday)

Time: 11:00 AM

Venue: FB421 (MSE conference room)

Zoom link:

https://iitk-ac-in.zoom.us/j/94549385413?pwd=QXNUZGVSRkdEZWU5T2pnQ3E2MVozZz09

Meeting ID: 945 4938 5413
Passcode: 505167

Abstract:

Single-walled carbon nanotubes (SWCNT) and single-layer graphene (SLG) are the most widely studied allotropes of sp2 hybridized carbon with unique properties owing to their one-dimensional and two-dimensional structures, respectively. In recent years, there has been a push to use mixed-dimensional heterostructures, such as the hybrids of SWCNT and SLG, for various applications which take the benefits of the unique properties of individual components while overcoming their limitations. Hybrid carbon nanostructures based on SWCNT and SLG hold vast potential for applications in electronics of various forms. In general, the properties of such hybrid structures are modified due to the interaction between the atoms of the components, and a constitutive understanding of these interactions can be utilized to tailor the properties of these hybrid structures to suit different applications.

The interactions between SWCNT and SLG in their hybrid nanostructures can be of various forms, such as the electronic interaction at the interface, the van der Waal's (vdW) forces between the atoms of the two components, and the localized structural deformations in the component structures which are eventually caused by the vdW forces. These factors are known to affect the vibrational, electronic, and transport properties of the isolated SWCNT and SLG in terms of shifts in their Raman active vibrational frequencies, modified electronic structure, and therefore influencing the electronic transport through these materials. The work presented in this thesis mainly focuses on the computational study of these interactions between SWCNT and SLG in their hybrids and the effects of these interactions on the structural, vibrational, electronic, and transport properties have been explored in various hybrid systems of SLGs with semiconducting and metallic (both achiral and chiral) SWCNTs using the density-functional tight-binding (DFTB) method.

We have investigated the role of various interactions on the structural and vibrational properties of the hybrid nanostructures. The changes in vibrational properties are deconvoluted to chart the effect of individual factors responsible for causing shifts in Raman active mode frequencies. From our calculations, it is apparent that structural deformation and vdW forces are the main factors affecting the vibrational

properties of components within the hybrid, with structural deformation being the dominant factor. It has been observed that the extent of charge transfer between SWCNT and SLG at the vdW separation (~3 Å) is not sufficient to cause any significant changes to the Raman active phonon frequencies of the components. With a decrease in separation, the magnitude of the charge exchanged between the components increases, however, the resultant vdW forces increase very rapidly and therefore remain the major factor to cause changes in vibrational properties.

The electronic properties of SWCNT-SLG hybrid nanostructures are investigated using the DFT (density functional theory) and DFTB methods by analyzing hybrid systems with both semiconducting and metallic SWCNTs (both chiral and achiral) to propose a general behavior. In this work, we demonstrate that the electronic structure of these hybrid systems are mainly modified (with respect to the pristine components) due to the electronic interactions between the components with negligible changes caused by the vdW forces and structural deformations. This electronic interaction leads to the mixing of electronic bands of SWCNT and SLG at energies where these bands cross each other and modify the band structure in terms of flattening, separation (breaking of degeneracy), and a decrease in curvature of the energy bands and opening of sub-band gaps, which in turn affects the transport properties of these hybrid nanostructures. The major contribution towards the electronic bands around the Fermi energy comes from the 2p orbitals of the carbon atoms. The effect of the electronic interaction further increases with decreasing separation between the components as reflected in the increasing flattening (decreasing curvature) of the bands, increasing sub-band gaps, and an increasing density of states (DOS) and partial density of states (PDOS) of the components with decreasing separation. Due to the highly localized interaction between SWCNT and SLG at the heterojunction, only locally interacting atoms of the components contribute to the total DOS at higher separations (higher than the vdW separation), whereas, at smaller separations, the neighboring atoms around the junction area also contribute significantly.

Further, we demonstrate how the electronic interaction between SCWNT and SLG affects the electronic transport through their hybrid nanostructures. The electronic transport properties of these hybrid nanostructures (again with both semiconducting and metallic SWCNTs) are calculated using the NEGF (non-equilibrium Green's function) transport formulation in combination with the DFTB method. At the vdW separation between the components, the drain current in the hybrids is found to be smaller than the sum of component currents at all source-drain biases. The smaller current in hybrids is a consequence of the modified electronic structure caused by the interactions between the components and this is true for hybrids with both semiconducting and metallic SWCNTs. With decreasing separation between the components, the drain current in hybrids with semiconducting SWCNTs (sc-SWCNT) increases at smaller source-drain biases, whereas the hybrid current decreases at higher source-drain biases. Unlike this, in hybrids with metallic SWCNTs (m-SWCNT), the drain current decreases with decreasing separation at all source-drain biases. The increase in current in hybrids with semiconducting SWCNT at lower biases is due to the decrease in an apparent gap in the local DOS close to the Fermi energy with a decrease in separation, whereas the decrease in current in hybrids with semiconducting SWCNT at higher biases and in hybrids with metallic SWCNT at all biases is a direct result of the changes in energy dispersion due to the electronic interaction between the components. In hybrid devices, the current can be modified at a given source-drain bias by applying an additional gate electrode and our calculations for such three-terminal devices show that higher modulation in the drain current can be achieved in the top-graphene configuration (gate applied on the graphene side) of the hybrid devices in comparison to the top-CNT configuration (gate applied on the CNT side) with varying gate voltage. Additionally, the screening of the gate potential by one component of the hybrid (closer to the gate electrode) on the other component (away from the gate electrode) is also observed in these three-terminal devices. In the top-CNT configuration, the strength of the screening effect due to metallic SWCNTs on SLG is higher than the semiconducting SWCNTs, whereas the screening effect due to SLG on both types of SWCNTs in the top-Gr configuration of the hybrids is approximately similar. The strength of the electric field screening effect of the three components (the sc-SWCNT, the m-SWCNT, and the SLG) obey the following order: m-SWCNT > Gr > sc-SWCNT. Our results provide an insight into how the charges are transported in such hybrid systems and may also provide a way to design new sp2 carbon-based hybrid nanostructures with desired properties by utilizing the modifications in their electronic structure due to the inter-component interactions.

All interested are cordially invited to join in person (FB421) or online (via zoom).

With regards,

Anshu Gaur

(Thesis Supervisor)

Attachments:

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Size:	8.7 k
Type:	text/plain
