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ELECTRONIC AND PHOTONIC PROPERTIES OF TWO DIMENSIONAL MATERIALS

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The state-of-the-art bismuth photonics is currently a very active and progressive area of research, as bismuth optical circuits have emerged as a possible replacement technology for copper-based circuits in communication and broadband networks. The demand for ever-improving communications and computing performance continues, and this in turn means that photonic circuits are finding ever-increasing application areas. This final report provides an important and timely investigation of a `hot topic' in the field, covering an important aspect of the technology that forms the research area of bismuth photonics. Specifically, we have calculated the Landau levels in an external magnetic field in the presence of a vertical electric field using the generalized tight-binding model. Then, we obtained the density-of-states, Hall conductance, the magneto-optical absorption spectrum along with the selection rules, magnetoplasmons and the inelastic carrier lifetimes, taking account of the role played by strain and defects. We determined the stable adsorption position of Bi atoms in III-V semiconductors and obtain the energy band structures and the dependence of the energy gaps on the doping concentration. Additionally, we have investigated a new type of device transferring DC current energy into terahertz waves in Bi due to the instability of the plasmons in a hybrid plasmonic structure. Such a structure consists of a Bi layer, which is Coulomb-coupled to a thick or a finite-width conductor.

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TABLE OF CONTENTS

Section **Page**

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1 SUMMARY

The state-of-the-art bismuth photonics is currently a very active and progressive area of research, as bismuth optical circuits have emerged as a possible replacement technology for copper-based circuits in communication and broadband networks. The demand for ever improving communications and computing performance continues, and this in turn means that photonic circuits are finding ever increasing application areas. This proposal provides an important and timely investigation of a `hot topic' in the field, covering an important aspect of the technology that forms the research area of bismuth photonics. Specifically, we will calculate the Landau levels in an external magnetic field in the presence of a vertical electric field using the generalized tight-binding model. Then, we will obtain the density-of-states (DoS), Hall conductance, the magneto-optical absorption spectrum along with the selection rules, magnetoplasmons and the inelastic carrier lifetimes, taking account of the role played by strain and defects. We will determine the stable adsorption position of Bi atoms in III-V semiconductors and obtain the energy band structures and the dependence of the energy gaps on the doping concentration. Additionally, we will investigate a new type of device transferring DC current energy into terahertz waves in Bi due to the instability of the plasmons in a hybrid plasmonic structure. Such a structure consists of a Bi layer, which is Coulomb-coupled to a thick or a finite-width conductor.

2 INTRODUCTION

During the funding period, we have made considerable progress on several fronts and we have published our results in the leading journals in the field of condensed matter physics. We now briefly describe the highlights of our investigations.

When a graphene layer is subjected to mechanical strain, the underlying crystal structure is deformed, resulting in a modified energy band structure [1-7], its electrical and thermal conductivity [1,8], as well as other transport properties [9,10]. Additionally, its polarizability is altered, thus giving rise to qualitative changes in the plasmon dispersion relation. Making use of the polarization function derived in Refs. [1, 11-13] for strained graphene, we have investigated the plasmon mode dispersion for a layered structure which could now be adapted to one involving strained bismuthene. Furthermore, we analyzed the effect due to strain [14] on the plasmon mode dispersion relation for previously studied structures [15, 16] which are special cases of the hybrid heterostructure we formulated. We have obtained analytical and numerical results showing the effect due to strain and phonon vibrations in the substrate on the plasmon excitation spectrum in the long wavelength limit by varying several parameters including the angle giving the direction of the applied strain, the strain modulus, the separation between the graphene layers, the dielectric constant for the background material and the wave vector. This information will be useful in designing applications involving nanoelectronic and optoelectronic devices.

3 METHODS, ASSUMPTIONS, AND PROCEDURES

We have developed theoretical methods to investigate the fundamental physical properties of emergent two-dimensional (2D) structures, including their electronic properties. Layered condensed-matter systems have attracted considerable attention from both a theoretical and experimental point of view [17-22], mainly as a result of their nano-scaled thickness and their lattice symmetries. They are ideal 2D materials for studying novel physical, chemical and materials science properties. Furthermore, such systems have exhibited high potential for future technological applications, such as nano-electronics, optoelectronics, and energy storages. Our proposed research has focused on group-IV 2D systems, covering graphene, silicene, and germanene as well as group-V Bi and P. Such systems will play critical roles in both basic and applied science. The combined effects on the defect-enriched electronic properties were explored in detail using well-established modified theoretical models. The planar/buckled structure, the intralayer and interlayer atomic interactions, the spin-orbital couplings, the defect-dependent site energy, and the magnetic/electric field have been taken into account in our calculations.

The method for solving the Hamiltonian is one of the basic challenges we have to deal with in our investigation. The generalized tight-binding model, which is based on sub-envelope functions of different sublattices, has been developed to consider all the important mechanisms simultaneously, such as the single- or multi-orbital chemical bondings, the spin-orbit coupling (SOC), the magnetic field, the electric field, the composite fields, the intralayer and interlayer hopping integrals, the number of layers, the stacking configurations, the curved surfaces, the hybridized structures, and the dimensions [23-26]. This model is also suitable for including the defect-dependent interactions in the Hamiltonian. The numerical challenge of diagonalizing a huge Hermitian matrix could be overcome by employing a band-like one. The defect configurations as well as the external fields have greatly diversified the electronic properties in terms of their band structure, valley and spin degeneracies, energy gap/band overlap, spatial probability distribution, and density-of-states.

4 RESULTS AND DISCUSSION

So far, previous investigations have shown that 2D group-IV systems exhibit rich and unique properties. Graphene has a sp_2-bonding planar structure, whereas germanene and silicene possess buckled structures with a mixed sp_2-sp_3 chemical bonding. Additionally, the spin-orbit coupling is significant in the low-energy electronic properties of the latter two. Monolayer graphene, as confirmed from many experimental measurements, presents a novel Dirac-cone band structure. The massless Dirac fermions mainly arise from a honeycomb lattice with a high geometric symmetry. This structure is an unusual gapless semiconductor with a vanishing density-of-states at the Fermi level. Silicene and germanene belong to direct-gap semiconductors, since the Dirac cones are distorted and separated by the SOC. Specially, both valley and spin degeneracies are revealed in all the group-IV systems. The breaking of state degeneracy could be achieved by modulating the lattice symmetries and applying external fields. This can promote further investigations on the valley- and/or spin-dominated electronics.

The manipulation of an energy band gap, being directly related to semiconducting properties, can diversify the main electronic properties. An efficient way is to utilize the effects due to defects. Various defects are frequently produced during fabrication. These include vacancies, substituted atoms, extra adatoms on the surface, and distorted lattices. There are only a few theoretical predictions on the defect-enriched properties of graphene systems. We have already begun work on defect-related silicene, germanene graphene and bismuthene. For such systems, the defects can the destroy lattice symmetry, distinct site energies (the change of the ionization potential), and non-uniform atomic interactions (the position-dependent hopping integrals). The dependences of the electronic properties on the type, distribution and concentration of defects are worthy of a detailed investigation. For example, whether the semiconductor-semimetal transition, the localization of wave functions, and the valley- and spin-split states could appear under the various defect configurations. Moreover, the complicated cooperative/competitive relations among the combined effects are proposed to comprehend the diverse electronic properties.

Electric and magnetic fields can dramatically modify the defect-dependent electronic properties. The main effect of the former is to drastically change the Coulomb potentials experienced by all the periodic atoms. However, the defects induce a local variation of the Coulomb potential. As for silicene and germanene with Spin-Orbit Coupling (SOC's), an electric field can destroy the x-y-plane mirror symmetry and thus create the valley- or spin-split states. Apparently, the composite effects due to defect and electric field will result in unusual electronic properties. It is well known that a uniform perpendicular magnetic field creates highly degenerate Landau levels (LLs) by quantization of the neighboring electronic states. The well-behaved LLs possess symmetric/antisymmetric probability distributions in a localized range, and their energy spectra exhibit the band-dominated field dependences. There exists a strong competition between magnetic field and defects since the latter induce a non-uniform environment. The defects might have a strong effect on the magnetic quantization, such as, the distortions and mixings of the LL wave functions, the changes of the localization ranges, the reduced LL state degeneracy, and the irregular field-dependent energy spectra (the crossing and anti-crossing behaviors).

Our major achievements have been summarized as follows:

(1) In our work [10], the combined effect due to mechanical strain, coupling to the plasmons in a doped conducting substrate, the plasmon-phonon coupling in conjunction with the role played by encapsulation of a secondary two-dimensional (2D) layer is investigated both theoretically and numerically. The calculations are based on the random-phase approximation (RPA) for the surface response function which yields the plasmon dispersion equation that is applicable in the presence or absence of an applied uniaxial strain. We present results showing the dependence of the frequency of the charge density oscillations on the strain modulus and direction of the wave vector in the Brillouin zone. The shielding of a dilute distribution of charges as well as the rate of loss of energy for impinging charges is investigated for this hybrid layered structure.

(2) In our work [27], the generalized tight-binding model is developed to investigate the rich and unique electronic properties of AB-bt (bottom-top) bilayer silicene under uniform perpendicular electric and magnetic fields. The first pair of conduction and valence bands, with an observable energy gap, displays unusual energy dispersions. Each group of conduction/valence Landau levels (LLs) is further classified into four subgroups, i.e., the sublattice- and spin-dominated LL subgroups. The magnetic-field-dependent LL energy spectra exhibit irregular behavior corresponding to the critical points of the band structure. Moreover, the electric field can induce many LL anticrossings. The main features of the LLs are uncovered with many van Hove singularities in the density-of-states and nonuniform delta-function-like peaks in the magnetoabsorption spectra. The feature-rich magnetic quantization directly reflects the geometric symmetries, intralayer and interlayer atomic interactions, spin-orbital couplings, and field effects. The results of this work can be applied to novel designs of Si-based nano-electronics and nano-devices with enhanced mobilities.

(3) In our work [28], the rich and unique magnetic quantization phenomena of Si-doped graphene defect systems for various concentrations and configurations are fully explored by using the generalized tight-binding model. The non-uniform bond lengths, site energies and hopping integrals, as well as a uniform perpendicular magnetic field (B_z $\mathbf{z}_0$) are taken into

account simultaneously. The quantized Landau levels (LLs) are classified into four different groups based on the probability distributions and oscillation modes. The main characteristics of the LLs are clearly reflected in the magneto-optical selection rules which cover the dominating $n = |n^v - n^c| = 0$, the coexistent $n = 0$ and $n = 1$, along with the specific $n = 1$. These rules for inter-LL excitations are attributed to the non-equivalence or equivalence of the Ai and Bi sublattices in a supercell. The spectral intensity can be controlled by oscillator strength using a canonical momentum (vector potential) as well as by density of states using concentration and distribution of doped Si atoms.

(4) In our work [29], we conduct a comprehensive investigation of the effect of an applied electric field on the optical and magneto-optical absorption spectra for AB-bt (bottom-top) bilayer silicene. The generalized tight-binding model in conjunction with the Kubo formula is efficiently employed in the numerical calculations. The electronic and optical properties are greatly diversified by the buckled lattice structure, stacking configuration, intralayer and interlayer hopping interactions, spin-orbital couplings, as well as the electric and magnetic fields ($E_z\,\mathbf{z}_0$ & $B_z\,\mathbf{z}_0$). An electric field induces spin-split electronic states, a semiconductor-metal phase transitions and the Dirac cone formations in different valleys, leading to the special absorption features. The E_z-dependent low-lying Landau levels possess lower degeneracy, valley-created localization centers, peculiar distributions of quantum numbers, well-behaved and abnormal energy spectra in B_z-dependencies, and the absence of anti-crossing behavior. Consequently, the specific magneto-optical selection rules exist for diverse excitation categories under certain critical electric fields. The optical gaps are reduced as E_z is increased, but enhanced by B_z, in which the threshold channel might dramatically change in the former case. These characteristics are in sharp contrast with those for layered graphene.

(5) In our work [30], the magneto-optical properties of bilayer phosphorene is investigated by the generalized tight-binding model and the gradient approximation. The vertical inter-Landau-level transitions, being sensitive to the polarization directions, are mainly determined by the spatial symmetries of sub-envelope functions on the distinct sub lattices. The anisotropic excitations strongly depend on the electric and magnetic fields. Perpendicular uniform electric field could greatly diversify the selection rule, frequency, intensity, number and form of symmetric absorption peaks. Specifically, the unusual magneto-optical properties appear beyond the critical field as a result of two subgroups of Landau levels with the main and side modes. The rich and unique magneto-absorption spectra arise from the very close relations among the geometric structures, multiple intralayer and interlayer hopping integrals, and composite external fields.

5 CONCLUSIONS

The generalized tight-binding model can combine with the many- and single-particle theories, when the latter are expressed in the sublattice-dominated forms [23-26]. The combined models are suitable for studying the other essential properties, such as the Coulomb excitations, transport properties, and optical spectra. The modified random-phase approximation is further utilized to explore the defect-enriched electron-electron interactions, e.g., the diversified electron-hole excitations and plasmon modes (phase diagrams). The combination with the static Kubo formula is useful in understanding the quantum Hall transport properties, e.g., the defect effects on the existence, height and field-dependence of the quantized conductivity. Moreover, the dynamic Kubo formula can be used to examine whether there exist distinct magneto-optical selection rules under the various defect configurations. In short, it is worthy of a thorough investigation on the essential properties of group-IV 2D systems.

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LIST OF ACRONYMS, ABBREVIATIONS, AND SYMBOLS

DOS	Density-of-States
2D	Two Dimensional
SOC	Spin-Orbit Coupling
LLs	Landau Levels
RPA	Random-Phase Approximation

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