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Defect-enriched electronic properties of group-IV 2D systems

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14. ABSTRACT
The PI investigated the rich magneto-electronic properties of AA-bottom-top (bt) bilayer silicene using a generalized tight-binding model. The electronic structure exhibits two pairs of oscillatory energy bands in which the lowest conduction and highest valence states of the low-lying pair are away from the K point. The quantized Landau levels (LLs) are classified into various separated groups by the localization behaviors of spatial distributions. The LLs in the vicinity of Fermi energy do not present simple wave function modes which are quite different from other two-dimensional systems. The geometry symmetry, intralayer and interlayer atomic interactions, and effect of a perpendicular magnetic field are responsible for the peculiar LL energy spectra in AA-bt bilayer silicene. In the PIs work, they provide a better understanding of the diverse magnetic quantization phenomena in 2D condensed-matter materials.

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2D Layered Materials, Group IV Semiconductor, semimetal phase transition, tight binding model

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Abstract: This work is focused on the defect-enriched electronic properties of group-IV 2D systems. The dependence on the type, distribution and concentration of defects and the interplay with the magnetic and electric fields are explored in detail. We will develop the generalized tight-binding model to include the defect-dependent interactions and the external fields in the Hamiltonian simultaneously. The defects might induce the valley- and spin-split electronic states, the semiconductor-semimetal transition, and the localization of wave function. They are expected to have strong effects on the magneto-electronic properties, covering the reduced Landau-level degeneracy, the unusual magnetic-field-dependent energy spectra, and the drastic change of quantum oscillation modes.

Introduction: We will develop theoretical models to investigate the essential physical properties of 2D emergent systems, especial for the electronic properties. Layered condensed-matter systems have attracted a lot of theoretical and experimental studies [R1-R6], mainly owing to their nano-scaled thickness and their rich lattice symmetries. They are ideal 2D materials for studying the novel physical, chemical and material phenomena. Furthermore, such systems have displayed high potentials for future technological applications, e.g., nano-electronics, optoelectronics, and energy storages. This proposed work is focused on group-IV 2D systems, covering graphene, silicene, and germanene. Such systems will play critical roles in the basic and applied sciences. The combined effects on the defect-enriched electronic properties could be explored in detail by using modified established 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 will be taken into account in our calculations.

Up to now, the previous studies had shown that 2D group-IV systems exhibit rich and unique essential properties. Graphene has a sp2-bonding planar structure, while germanene and silicene possess the buckled structures with a mixed sp2-sp3chemical bonding. Furthermore, 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 system 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 studies on the valley- and/or spin-dominated electronics.

The engineering of an energy gap, being closely related to semiconductor applications, can diversify the main features of electronic properties. One of the efficient ways is to utilize the defect effects. Various defects are frequently produced during experimental syntheses, e.g., the vacancies, substituted atoms, extra adatoms on surface, and distorted lattices. There are only a few theoretical predictions on the defect-enriched properties of graphene systems. The defect-related silicene, germanene and graphene will be chosen for a model study. For such systems, the defects can create

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the destruction of lattice symmetry, the distinct site energies (the change of the ionization potential), and the 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 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).

Experiment: The method for solving the Hamiltonian is one of the basic challenges in theoretical physics. 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 distinct dimensions [R7-R10]. 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 solved by using a band-like one. The defect configurations and the external fields are expected to greatly diversify the electronic properties in terms of the band structure, valley and spin degeneracies, energy gap/band overlap, spatial probability distribution, and density of states.

The generalized tight-binding model can combine with the many- and single-particle theories, when the latter are expressed in the sublattice-dominated forms [R7-R10]. 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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Results and Discussion:

PHYSICAL REVIEW B 97, 195302 (2018)

Coulomb scattering rates of excited states in monolayer electron-doped germanene

Po-Hsin Shih, Chih-Wei Chiu, Jhao-Ying Wu, Thi-Nga Do, and Ming-Fa Lin

Excited conduction electrons, conduction holes, and valence holes in monolayer electron-doped germanene exhibit unusual Coulomb decay rates. The deexcitation processes are studied using the screened exchange energy. They might utilize the intraband single-particle excitations (SPEs), the interband SPEs, and the plasmon modes, depending on the quasiparticle states and the Fermi energies. The low-lying valence holes can decay through the undamped acoustic plasmon, so that they present very fast Coulomb deexcitations, nonmonotonous energy dependence, and anisotropic behavior. However, the low-energy conduction electrons and holes are similar to those in a two-dimensional electron gas. The higher-energy conduction states and the deeper-energy valence ones behave similarly in the available deexcitation channels and have a similar dependence of decay rate on the wave vector k.

PHYSICAL REVIEW B 97, 125416 (2018)

Diverse magnetic quantization in bilayer silicene

Thi-Nga Do, Po-Hsin Shih, Godfrey Gumbs, Danhong Huang, Chih-Wei Chiu, and Ming-Fa Lin

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 nanoelectronics and nanodevices with enhanced mobilities.

Carbon 144 (2019) 608-614

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Magneto-electronic and optical properties of Si-doped graphene
Po-Hsin Shih, Thi-Nga Do, Bor-Luan Huang, Godfrey Gumbs, Danhong Huang, and Ming-Fa Lin

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 ($\mathbf{B}_z\hat{\mathbf{z}}$) 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 $\Delta n = |n^v - n^c| = 0$, the coexistent $\Delta n = 0$ and $\Delta n = 1$, along with the specific $\Delta n = 1$. These rules for inter-LL excitations are attributed to the non-equivalence or equivalence of the A_i and B_i 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.

Scientific Reports **9**, 624 (2019)
Peculiar optical properties of bilayer silicene under the influence of external electric and magnetic fields
Thi-Nga Do, Godfrey Gumbs, Po-Hsin Shih, Danhong Huang, Chih-Wei Chiu, Chia-Yun Chen, and Ming-Fa Lin

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 ($\mathbf{E}_z\hat{\mathbf{z}}$ & $\mathbf{B}_z\hat{\mathbf{z}}$). 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 $\mathbf{E}_z$-dependent low-lying Landau levels possess lower degeneracy, valley-created localization centers, peculiar distributions of quantum numbers, well-behaved and abnormal energy spectra in $\mathbf{B}_z$-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 $\mathbf{E}_z$ is increased, but enhanced by $\mathbf{B}_z$, in which the threshold channel might dramatically change in the former case. These characteristics are in sharp contrast with those for layered graphene.

arXiv:1905.03983 (submitted to Sci. Rep.)
Diverse quantization phenomena in AA bilayer silicene
Po-Hsin Shih, Thi-Nga Do, Godfrey Gumbs, Danhong Huang, Hai Duong Pham, and Ming-Fa Lin

The rich magneto-electronic properties of AA-bottom-top (bt) bilayer silicene are investigated using a generalized tight-binding model. The electronic structure exhibits two pairs of oscillatory energy bands in which the lowest conduction and highest valence states of the low-lying pair are away from the K point. The quantized Landau levels (LLs) are classified into various separated groups by the localization behaviors of spatial distributions. The LLs in the vicinity of Fermi energy do not present simple wave function modes which are quite different from other two-dimensional systems. The geometry symmetry, intralayer and interlayer atomic interactions, and effect of a perpendicular magnetic field are responsible for the peculiar LL energy spectra in AA-bt bilayer silicene. This work provides a better understanding of the diverse magnetic quantization phenomena in 2D condensed-matter materials.

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List of Publications:

1. P. H. Shih, C. W. Chiu, J. Y. Wu*, T. N. Do, and M. F. Lin*, “Coulomb scattering rates of excited states in germanene.”, Phys. Rev. B 97, 195302 (2018).
2. T. N. Do, P. H. Shih, G. Gumbs, D. Huang, C. W. Chiu, and M. F. Lin*. “Diverse magnetic quantization in bilayer silicene.”, Phys. Rev. B 97, 125416 (2018).
3. P. H. Shih, Thi-Nga Do, B. L. Huang, Godfrey Gumbs, D. H. Huang, and M. F. Lin, “Magneto-electronic and optical properties of Si-doped graphene”, Sci. Rep. 144, 608 (2019)
4. T. N. Do, G. Gumbs, P. H. Shih, D. H. Huang, C. W. Chiu, C. Y. Chen, and M. F. Lin, “Peculiar optical properties of bilayer silicene under the influence of external electric and magnetic fields”, Sci. Rep 9, 624 (2019)
5. P. H. Shih, T. N. Do, G. Gumbs, D. Huang, H. D. Pham, and Ming-Fa Lin, “Diverse quantization phenomena in AA bilayer silicene”, arXiv:1905.03983.

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