Tunable electronic and magnetic properties of two-dimensional materials and their one-dimensional derivatives

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Low-dimensional materials exhibit many exceptional properties and functionalities which can be efficiently tuned by externally applied force or fields. Here we review the current status of research on tuning the electronic and magnetic properties of low-dimensional carbon, boron nitride, metal-dichalcogenides, phosphorene nanomaterials by applied engineering strain, external electric field and interaction with substrates, etc, with particular focus on the progress of computational methods and studies. We highlight the similarities and differences of the property modulation among one- and two-dimensional nanomaterials. Recent breakthroughs in experimental demonstration of the tunable functionalities in typical nanostructures are also presented. Finally, prospective and challenges for applying the tunable properties into functional devices are discussed. © 2016 The Authors. WIREs Computational Molecular Science published by John Wiley & Sons, Ltd.

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INTRODUCTION

The past two decades have seen a bloom of research activities in nanoscience and a rapid development in delivering the potential of nanotechnology into diverse applications. The major driving force for these activities and development is that nanoscale materials can offer novel electronic, magnetic, optical, mechanical, and chemical properties, which lead to distinguished performance in many technological fields, such as mechanic engineering, electronics, information, and energy technologies. The most intriguing behavior of nanomaterials is that their intrinsic properties are amenable to efficient modulation by applying various physical fields, in contrast to macroscopic systems.

In continuum, the functionality predominantly relies on the materials’ bulk properties and thus only a small number of materials have useful responses to applied physical fields. As the materials and devices scale down to nanoscale, the timescale can be down to nanosecond (10^{-9} s), pico-second (10^{-12} s), and even femto-second (10^{-15} s). Accordingly, the energy scale changes from Joule (N∙m) in macroscopic systems to 10^{-18} Joule (nN∙nm, aJ) in nanosystems, which approaches the level of electron-volt (eV), namely the characteristic energy scale of local fields constituted by charge, molecular orbits, electron spins, and structures. Therefore, the physical fields (e.g., strain, electric and magnetic fields and substrates) applied to nanomaterials is prone to a strong coupling with the local fields and thereby remarkably changes the properties of systems, as shown in Figure 1(a). At nanoscale, the coupling between local and external fields can be remarkable even in materials that are featureless in their bulk counterparts,^2

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hatching out a series of tunable properties and functionalities and offering a wealth of opportunities for the development of nanoscience and the innovation in nanotechnology.

In terms of dimensionality, nanomaterials can exist in forms of zero-dimensional (0D) nanoclusters and nanoparticles, one-dimensional (1D) nanowires, nanotubes and nanoribbons, two-dimensional (2D) atomic crystals and nanoﬁlms and 3D superstructures made of nanoscale components. In particular, the 1D and 2D nanomaterials, termed as low-dimensional materials, are the ideal systems for studying the peculiar nanoscale effects, which are of benefit not only for understanding fundamental phenomena under these dimensionalities but also for developing functional nanodevices with high performance. The 2D materials, represented by semimetallic graphene, insulating hexagonal boron nitride (h-BN) and semiconducting transition metal dichalcogenides MX_{2} family (M = Mo, W; X = S, Se), have attracted most research attentions during the past decade. Graphene, a single-layer of graphite, possesses a number of extraordinary properties owing to its Dirac-like band dispersion at the Fermi level, but it has no bandgap to enable logic operation.3 The h-BN monolayer, isostructural to graphene, is electrically insulating owing to the lack of inversion symmetry.4 Differently, the semiconducting 2D MX_{2} has metal-ligand bonding and a three-atom thickness, with the M atoms sandwiched between layers of X ligands. A notable technological advantage of these 2D materials is that they can be wrapped into cylindrical nanotubes and tailored into nanoribbons (Figure 2(a)). Quantum conﬁnement effects enrich the nanotubes and nanoribbons with even more fascinating functionalities and promise enhanced efﬁciency for electronic devices. Tuning the electronic and magnetic properties of these low-dimensional systems is always the object of extensive research, as tunable properties are highly desirable to allow great flexibility in design and optimization of functional devices. In this review, we focus on the mechano-electro-magnetic coupling effect and discuss the inﬂuence of strain, external electric ﬁelds and substrates on the electronic and magnetic properties of these materials (Figure 1(b)).

Since low-dimensional materials are structurally ﬂexible and easy to deform, strain proves to be effective to tune their properties. In nanomaterials, strain not only changes atomic conﬁgurations, but also modiﬁes the overlap of electron orbitals, charge distribution and bonding strength, providing a fertile ground for hatching novel properties. This behavior contrasts that of bulk materials where strain is related mostly simply to mechanical deformation. Nevertheless, the nanoscale strain effects differ from material to material and from 1D to 2D, and we are still in the dark about a universal mechanism for these effects in low-dimensional materials. Moreover, applied strain could also interplay with other physical quantities, such as electron spins in magnetic materials and electric polarization in polar materials, resulting in unusual piezomagnetic and piezoelectric effects. Achieving high efﬁciency and sensitivity for these effects is always pursued in related ﬁelds and calls for a development of current theoretical views.

Applying electric ﬁeld is another common way toward achieving tunable properties. This is particularly suitable for low-dimensional materials since strong electric ﬁelds (e.g. from gates or interfaces) with strength in order of V/nm are prevalent in

![Figure 1](image-url)
nanosystems. The electric field, either applied or built-in, can shift and split the energy levels of nanostructures, which, in turn, sensitively tunes the electronic structures. Also, external electric fields could drive charge transfer to electrically polarize the materials. In magnetic nanomaterials, the charge transfer alters the local spin population so as to modulate the magnetism of system. Moreover, the field-induced polarization can also couple to lattice structures, deforming the chemical bonds to induce electrostrictive effect. The progress on the electric field effects applies especially to theory-oriented works, while experimental research is still lingering behind. The major reason is that the involved electric field strength is too strong. Moreover, a great challenge remains in efficiently applying the fields to a target nanostructure. These issues stimulate further study of new principles and paradigms that are more feasible for achieving electric-field-tunable properties.

Strain and electric field effects in low-dimensional materials form the basis of mechano-electro-magnetic coupling at nanoscale. These effects enable precise control of material properties that is ideally suited for designing on-demand devices. While many exotic properties can stem from this nanoscale multiple-field coupling, they may be influenced by substrates or metal contacts that are unavoidable for device fabrication. Thus, fully understanding the impact of substrates on the material properties is also of central importance. The mechano-electro-magnetic coupling and substrate effects are essential for realizing functionality-oriented nanodevices. Toward this goal, experimentalists and theorists are required to make concerted efforts. Especially, for the sake of materializing many theoretically proposed concepts, it is important to improve the production and fabrication techniques that enable the realization of nanomaterials with atomic precision. In this contribution, we present a comprehensive state-of-the-art review on the tunable electronic and magnetic properties of low-dimensional materials and thoroughly summarize valuable achievements with respect to promising functionality modulation, novel device concepts, and prospective applications. We focus on 2D graphene and $h$-BN sheet and their 1D derivatives. Other newly emerged 2D materials, such as MX$_2$, phosphorene and MXenes will be accounted as well.
GRAPHENE NANOARCHITECTURES

Graphene

**Single-Layer Graphene**

Graphene exhibits many excellent properties, such as high electron mobility and long coherence length, due to a linear, Dirac-like energy dispersion near the Fermi level (Figure 2(b), left). The charge carriers in graphene behave as massless Dirac fermions that can be sensitively modulated by electric, magnetic, and strain fields. A major obstacle for graphene-based electronics is the inability to electrostatically confine electrons in graphene, which is semimetallic without a bandgap. There are primarily three ways toward opening a bandgap in graphene (Figure 2(b)). The first way is to tailor graphene into graphene nanoribbons (GNRs). A bandgap induced by quantum confinement effect can be opened in GNRs, whose edges can be further functionalized and shaped in various ways to achieve colorful properties. As will be reviewed later; yet an efficient bandgap that suffices to allow logic operation at room temperature requires the ribbon width to be less than 10 nm and the edges to be atomically smooth, which impose significant challenge on the fabrication. The second way is to form functionalized pattern in graphene by chemisorbing atomic species or forming antidot lattices. The bandgap opened in this way can be up to 3 eV but the electronic mobility of graphene is sacrificed to a large extent by unintended localized electronic states. The third way is to break the symmetry between two sublattices by putting graphene onto a solid substrate or applying electric fields to bilayer graphene. Electrically gated bilayer graphene allows a good trade-off between the high carrier mobility and acceptable bandgap and also benefits from being compatible with traditional device architectures.

Gap opening in graphene is also amenable to applied magnetic fields, under which the Dirac fermions undergo an energy quantization, manifested as a series of quantized Landau levels that can be expressed as

\[ E_i = \nu_F \sqrt{2eB|i} \]

where \( \nu_F \) is the Fermi velocity of graphene, \( B \) is the magnetic field strength and \( i \) is the index of the Landau levels. According to this expression, a vertical magnetic field of 45 T can open an energy gap of approximately 0.2 eV, which has been experimentally measured. The magnetic-field-induced unusual quantum phenomena in graphene, such as the relativistic quantum Hall effect and electron correlation effects, have been thoroughly discussed in a recent review. Of more interest is that the effect of vertical magnetic fields on the electronic properties of graphene can be mimicked by a distributed strain, which induces a pseudomagnetic field. Being designed to smoothly vary on the atomic scale, the strain deforms the Brillouin zone and shifts the Dirac cones away from the zone vertices (similar effect exists in carbon nanotubes (CNTs), as discussed later), resembling the effect of magnetic field induced on the charge carriers in graphene. Analytically, a 2D strain field leads to gauge-field vector potential \( A \), which yields a pseudomagnetic field as

\[ B = \partial A_y / \partial x - \partial A_x / \partial y, \]

where \( A \) is expressed as a tensor of strain gradient. Recent theories predicted a pseudomagnetic field of 10 T in graphene strained with triangular symmetry and of 160 T in twisted GNRs hundreds of nanometers wide. It has been experimentally reported that highly strained nanobubbles in graphene can induce a pseudomagnetic field greater than 300 T. However, unlike a real magnetic field, the pseudomagnetic field does not break the time reversal symmetry in graphene since the strain-induced gauge-field vector potential always has opposite sign at the two graphene valleys (at \( K_1 \) and \( K_2 \) of the Brillouin zone).

In contrast to the effect of nonuniform strain, graphene can persist with its semi-metallic nature under a uniform isotropic strain up to 25% or under a uniform shear strain up to 10% as these uniform strains cannot break the graphene inversion symmetry. Yet, uniaxial strain can bring evident anisotropy to the Fermi velocity of graphene, and, meanwhile, substantially increases the work function of graphene due to the raised vacuum level.

**Bilayer Graphene**

Bilayer graphene is special in that it can open a bandgap under applied vertical electric fields. The electrically tunable bandgap only exists in Bernal (AB)-stacked bilayer graphene, rendering the controlled synthesis of high-quality bilayer graphene highly appealing. In an electrically gated bilayer graphene, the measured carrier mobility reaches approximately 1000 cm² V⁻¹ s⁻¹ and the opened bandgap is up to 0.25 eV (Figure 3(a) and (b)). The electronic properties of bilayer graphene are very sensitive to interlayer coupling. Guo et al. reported by \textit{ab initio} calculations surprisingly high sensitivity of the field-induced bandgap of bilayer graphene to the change in interlayer spacing (Figure 3(c) and (d)): a 10% compression of the spacing enhances...
the field-induced bandgap by 80% under a moderate field strength, suggesting that the electric-field-induced asymmetry in bilayer graphene can be enhanced by nanomechanical modulation. When epitaxially grown on a substrate, as in most device applications, bilayer graphene exhibits new behaviors due to interactions with substrate. The bottom layer chemically interacts with the substrate by hybridizing its π state with dangling bonds of the substrate,\textsuperscript{13,27,28} whereas the top layer is usually n-doped due to charge transfer from the bottom layer and substrate. Structural defects or interlayer interaction with the bottom layer can open a small bandgap at the Dirac point of the top layer.\textsuperscript{13} Further, applying bias voltage to bilayer graphene on C-terminated SiC substrate could induce a n-to-p-type transition, and vertical compression leads to an increase of the bandgap of the top layer.\textsuperscript{29}

**FIGURE 3** Electrically tunable bandgap in bilayer graphene. (a) Schematic illustration of a side view of the electrically gated bilayer graphene. (b) Bandgap opened in graphene bilayer as a function of effective field strength. Theoretical results from self-consistent TB and \textit{ab initio} methods are compared with experiments. (Reprinted with permission from Ref 25 Copyright 2009 Nature). (c) Bandgap as a function of the field strength at different interlayer spacings $d$. The gray line on the left side of the curves indicates a universal linear scaling of the gap at low fields (below 0.3 V/nm) with a slope of 0.294 eV per V/nm for $d \leq 0.4$ nm. (d) Bandgap as a function of $d$ at different electric fields. The shaded/clear regions on the left/right side correspond to compression/expansion of the spacing $d$ from the equilibrium 0.334 nm. The inset in (d) shows the variation of interlayer force. (Reprinted with permission from Ref 26 Copyright 2008 American Institute of Physics).

**GNRs**

GNR, a strip of graphene of nanometers in width (Figure 2(a)), exhibits richer properties and behaviors because of its edge states and width effects. GNRs with armchair edges (AGNRs) are semiconducting, mainly attributed to quantum confinement effect; GNRs with zigzag edges (ZGNRs) show magnetic edges states, which induce a staggered sublattice potential on the hexagonal lattice and result in a bandgap near the Fermi level.\textsuperscript{7} The peculiar edge magnetism of ZGNRs has been experimentally confirmed, evidenced by a sharp change in the width-dependent bandgap in ZGNRs settled on a Cu substrate.\textsuperscript{30} In reality, the edges of GNRs often show roughness, with many atomic steps protruded out of the edges.\textsuperscript{31} Electronic and magnetic properties of the GNRs with periodic protruded edges are shown to depend on the length of the protruded step and step-
to-step distance along the ribbon edge.\textsuperscript{32} With a small step length, the GNR evolves from a nonmagnetic semiconductor, via metal, to a magnetic semiconductor with increasing inter-step distance. Electronic transport study of GNRs with edge irregularity showed that the edge roughness increases the minimal leakage current due to the localized states induced in the bandgap and decreases the on current due to smaller quantum transmission,\textsuperscript{33} from which, however, a transistor switching behavior is survived.

**Tunable Magnetism in GNRs**

Tuning the electronic and magnetic properties of GNRs is of special interest from both fundamental and technological perspectives. The ZGNRs have been intensively studied in this aspect. Applying transverse electric field (Figure 4(a)) or decorating the edges with different chemical groups is predicted to make half-metal from ZGNRs.\textsuperscript{34,37,38} Still, there is no experimental support to the half-metallic ZGNRs. The major issues contain: (1) the magnetic state in ZGNRs is very sensitive to edge quality and termination; (2) the magnetism is relatively weak and easy to be quenched by thermal activation; (3) it is challenging to effectively apply a strong electric field required for the half-metal to a target ZGNR. Very recently, Yu et al. proposed a new paradigm (Figure 4(b)) that can realize the half-metal in ZGNRs by applying bias voltages. They sandwiched a ZGNR between two h-BN nanoribbons (BNNRs); then applied bias voltage or vertical compression can tune the system into half-metal,\textsuperscript{35} due to increased electric polarization by the h-BN layers which enhances the exchange potential across the GNRs.

The semiconductor to half-metal transition can also be induced in bilayer GNRs. Guo et al. found that a bilayer ZGNR with antiferromagnetic coupling...
between the opposite edges can be tuned into half-metal by applying transverse electric field or strain.\textsuperscript{39} The bandgap of a bilayer ZGNR decreases with decreasing interlayer spacing until it is closed. To promote applications, Zhang et al. placed the bilayer ZGNR on silicon substrate and found tunable magnetoelectric effect (Figure 4(c)).\textsuperscript{36} They showed that an applied bias voltage drives charge transfer between the nanoribbons and substrate, which controls the exchange splitting of magnetic edge states and hence the edge magnetic moment. In particular, the bias induced \( n \)-to-\( p \)-type transition in the top ribbon layer can switch the magnetoelectric coefficient from negative to positive. For a monolayer ZGNR adsorbed on Si(001) substrate, the edge magnetism completely disappears due to the formed Si–C bonds at ribbon edges\textsuperscript{30}; yet the ZGNR can be semiconducting or metallic depending on the ribbon width and adsorption orientation. These findings pave the way for fabricating graphene-based electronic and spintronic devices by integrating with existing silicon technology.

**Strain Effect in GNRs**

The electronic structure of GNRs is tunable by strain. Theoretical studies showed that the electronic properties of ZGNRs are insensitive to uniaxial strain, while the bandgap of AGNRs changes in a zigzag pattern with uniaxial strain.\textsuperscript{41,42} This stands in stark contrast to graphene, whose semimetallic nature can persist at a uniaxial strain up to 25\%.\textsuperscript{21} In addition, twisting AGNRs can also couple the conduction and valence bands and linearly modulate the bandgap, with the slope of gap versus twist angle depending on the ribbon width.\textsuperscript{43} Moreover, in suspended GNRs, twisting couples with axial tensional strain and therefore leads to larger modulation of bandgap that manifests as a nonlinear function of twist angle.\textsuperscript{44} The underlying physics for the strain-tunable bandgap in AGNRs is similar to that in CNTs, since the bandgaps in both CNTs and AGNRs essentially share the same origin that is due to the quantized momentum along the transverse or circumferential direction (see related discussion on CNTs later). The electromechanical responses in the AGNRs could be exploited in switches and sensor applications.

**CARBON NANOTUBES**

**Basic Properties**

**Single-Walled CNTs**

CNTs were first characterized by Iijima in 1991 using electron microscopy.\textsuperscript{35} A single-walled CNT (SWCNT) is geometrically made up by rolling a graphene sheet into a cylinder along a specific direction. The structure of a SWCNT can be characterized by a chiral vector, \( \mathbf{C}_h = n \mathbf{a}_1 + m \mathbf{a}_2 \), or a chirality index \((n,m)\), where \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) are two basic vectors of graphene lattice. SWCNTs with a specific chirality have been realized by controlled synthesis methods.\textsuperscript{46,47} The chiral angle \( \theta \) can be obtained by \(\sin \theta = \sqrt{3} m/(2(m^2 + mn + n^2))\). Armchair and zigzag CNTs correspond to \( \theta = 30^\circ \) and \( 0^\circ \), respectively, as shown in Figure 5(a). The CNT diameter can be geometrically expressed as \( D = a/(n^2 + mn + m^2)/\pi \), where \( a \) is the lattice constant of graphene. In early CNT synthesis, the CNT diameter can vary from hundreds of nanometers to sub-nanometer. In 2000, small CNTs with diameters of 0.5\textsuperscript{49} and 0.4 nm\textsuperscript{50} were reported. Meanwhile, Peng et al. observed a small SWCNT with diameter of 0.33 nm, which exists as a tiny branch on a parent CNT.\textsuperscript{51} Three years later, Zhao et al. observed a 0.3-nm-diameter \((2, 2)\) CNT as the innermost wall of a multi-walled CNT (MWCNT),\textsuperscript{52} which should be the smallest CNT reported thus far. Along the longitudinal dimension, the longest CNTs can reach 2 mm in 1998\textsuperscript{53} and recently this record was updated to 550 mm,\textsuperscript{54} rendering the CNTs a bridge connecting the nanoscale matters to the macroscopic world.

**Multi-Walled Carbon Nanotubes**

A MWCNT is comprised of two or more concentrically aligned SWCNTs, being either periodic or aperiodic depending on the interwall commensurability. An important topic on MWCNTs is the chirality correlation of different tube walls. A number of experiments using different synthesis methods yield MWCNTs with identical or nearly identical chiralities when the growth temperatures are relatively low.\textsuperscript{55-57} Using molecular dynamics simulations with chirality-related potential, Guo et al. found\textsuperscript{58} that, for a MWCNT with a diameter more than 12 nm, nearly identical chiralities correspond to the energy optimum; for a MWCNT with diameter less than 10 nm, the chiral angle ratio of the outer to inner walls decreases with decreasing tube diameter, and the nearly identical zigzag chiralities are preferred when the tube diameter becomes very small.

**Electronic Structures of Carbon Nanotubes**

Understanding electronic structures of CNTs needs to start from graphene, which has a zero bandgap with the valence and conduction bands met at two vertexes of the Brillouin Zone, \( K_1 \) and \( K_2 \) (Figure 5(b)). The dispersion around the vertex is a cone.
Upon wrapping into a CNT, the electronic wave vector in the circumferential direction, $k_c$, is quantized and satisfies a boundary condition $\pi Dk_c = 2\pi j$, where $j$ is an integer; the as-allowed values of $k_c$ are represented by the horizontal lines in Figure 5(b) that miss $K_1$ or $K_2$ by an amount $\Delta k_c$. The CNT electronic structure near the Fermi level is determined by the Conic section of the dispersion cones by allowed $k_c$ (Figure 5(c)). When $n-m$ is a multiple of 3, $\Delta k_c = 0$, thus the corresponding CNT is metallic; otherwise it is a semiconductor. The energy distance between the upper and lower branches of the Conic section defines the CNT’s bandgap. The semiconducting CNT has its bandgap decreasing with increasing tube diameter $D$ and in the limit of $D \to \infty$ it converges to the semi-metallic graphene. When $D < 0.5$ nm, all CNTs become metallic independent of chirality due to curvature-induced rehybridization of $\sigma$ and $\pi$ orbitals.

In mechanical aspect, a pristine SWCNT possesses an extremely high elastic modulus over 1 TPa$^{60,61}$ comparable to that of diamond. A SWCNT can also withstand >12% tensile strain, two orders higher than that of steel. The tensile strength of CNTs can range from 20 to 63 GPa$^{62}$ depending on diameter while the compressive strength can reach up to 100 GPa$^{63}$. In the radial direction, CNTs are rather flexible and the compressive strength is estimated to be over 5.3 GPa$^{64}$. However, CNTs usually contain defects, such as dislocation (517) defects, vacancies, or impurities, which can dramatically influence the electronic and mechanical properties of CNTs. For example, a 517 defect can produce two quasi-bound states and reduce the conductance by one quantum unit at the corresponding energy.$^{65}$ The tensile strength can degrade to 60% of the ideal value in the presence of vacancies.$^{66}$

**Mechano-Electro-Magnetic Coupling Effect in Carbon Nanotubes**

**Electromechanical Coupling**

SWCNTs can be subject to various deformations, which are able to induce remarkable electromechanical coupling. As discussed, the electronic structure of a SWCNT is determined by chirality-dependent position of quantized wave vectors $k$ (along the tube circumference) relative to the Fermi point $k_F$ at $K_1$ and $K_2$. Applied uniaxial and torsional strains shift the Fermi point away from the $K_1$ and $K_2$, change $|k-k_F|$ or $\Delta k_c$ and thus modify the bandgap of CNTs.

![Figure 5](image-url)
The electronic structure of deformed CNTs depends on the chirality and deformation mode, which can be well described by the Hückel tight-binding (TB) model. The Hamiltonian matrix element for an undeformed SWCNT is given by:

\[ H_{ij}(\xi) = H_{ij}^0 \left( \tau_j \exp(i\Delta r_j) \right) \]

where \( \xi \) represents a 2D strain tensor, \( \Delta r_j \) is the deformation of the jth bond, and \( H_{ij}^0 \) is the Hamiltonian matrix element for an undeformed SWCNT. From this model, the change of CNT bandgap versus strain exhibits a zigzag pattern, with a periodicity reversely proportional to the tube diameter (Figure 6(c)). Specifically, the bandgap of zigzag CNTs is most sensitive to uniaxial strain yet most impervious to torsional strain; the opposite holds for the armchair CNTs. The strain-tunable bandgap of CNTs was confirmed in subsequent experiments, which showed that a uniaxial strain can open a bandgap in a metallic CNT and increase the electric resistance of CNTs (Figure 6(d)). The strong electromechanical coupling in CNTs has opened potential applications for nanoelectromechanical devices.

Compared to high axial stiffness, a SWCNT is much more flexible in the radial direction and prone to radial deformations. Early in 1999, Park et al. reported with \textit{ab initio} calculations that the CNT bandgap can be easily opened or closed by radial deformations. Later on, using a TB molecular dynamics, Lu et al. found a metal-to-semiconductor transition in squashed armchair CNTs, attributed to a combined effect of broken mirror symmetry and bond formation between flattened regions of tube wall. In 2005, a more
conclusive analysis on the squashed armchair CNTs was performed by Mehrrez et al., showing that the squashed armchair CNTs can restore to metallic at sufficiently high deformation even if the CNTs undergo a breaking of mirror symmetry, thanks to strong $\pi-\sigma$ hybridization. A metal–insulator CNT junction can be designed via local collapse of the nanotubes by, for example, depositing insulating layers. In addition, CNTs are easy to bend, in either local or uniform manner. The local bending leads to the mixing of $\sigma$ and $\pi$ states yet without gap opening in metallic CNTs. The electronic transport through a locally bent CNT is essentially unaffected unless the bending is large enough to introduce backscattering to decrease the conductivity. In contrast, a uniform bending is large enough to introduce backscattering locally.

The electronic transport through a metallic CNT lattices. First, electric fields strongly affect the structure and strength of CNTs. Several theoretical studies showed that the CNT failure under electric fields and modifies the bandgap, depending on the chirality as analyzed by Chibotaru et al. Transport study also supported that uniform bending decreases the conductivity through a metallic CNT but increases that through a semiconducting CNT, as the bending becomes severer, kink structures appear at the inner side of the CNT and break the monotonic dependence of the conductivity on deformation.

The electromechanical coupling can also manifest as the interaction between electric fields and CNT lattices. First, electric fields strongly affect the structure and strength of CNTs. Several theoretical studies showed that the CNT failure under electric fields or charge preferentially occurs at tube ends, to which adding caps can enhance the nanotube stability. Under a tensile load, Guo et al. found that the CNT breaks near its middle and its critical tensile strength declines significantly with increasing field strength. Subsequent experiments confirmed these theoretical results and further showed that the tube failure could also occur at defects on the tube wall. On the other hand, the mechanical and electric behaviors are always coupled with each other in CNTs. The design of CNT nanomemory is just based on the coupling of mechanical bending and electrostatic attraction. Under applied electric fields, the charge density in a CNT will be redistributed because of electric polarization near the ends so that the tube is locally not electrically neutral. This in turn causes the CNT to be stretched by electric fields. However, the CNT electronic structures, following a metal–insulator transition depending on tube diameter and chirality (Figure 6(e)). The giant electrostrictive deformation, together with the high stiffness of CNTs, opens a promising prospect for developing high-efficiency energy conversion devices. Another behavior worth mentioning is that CNTs can stretch (by ~1%) upon charge injection, contributed by a uniform deformation of C–C bonds due to the change in the population of electron orbitals. CNT actuators and sensors have been designed based on this effect.

Electromagnetic Coupling in Carbon Nanotubes

In CNTs, the electron and hole sub-bands have 1D feature, and their electronic states resemble semiclassical electron orbits encircling the nanotube. An electron moving along these orbits has an orbital magnetic moment $\mu_{orb}$ expressed as $\mu_{orb} = |e|V_F A/4$, where $V_F$ is the Fermi velocity of electrons. According to Zeeman effect, an applied axial magnetic field can shift the energy of sub-bands by $\Delta E = -\mu_{orb} B = \pm |e|V_F B/4$. This equation provides a simple relationship between the CNT bandgap and the magnetic field strength and accounts for experimental observations of giant magnetoresistance and metal–insulator transition in CNTs under axial magnetic fields. However, this equation cannot give the detailed electronic structures of CNTs under a magnetic field, which are necessary for understanding other important magnetic properties, such as magnetic susceptibility. For this purpose, the effective-mass approximation and TB model have been employed. Since the effective-mass approximation is valid only at the charge-neutral state and only provides the information about the electronic states near the Fermi level, we focus on the progress based on the TB model. For a CNT under a magnetic field with strength $B$, the vector potential is $A = (\phi/|C_0|, 0)$, where $\phi$ denotes the magnetic flux threading the CNT. Accordingly, the single-orbital nearest-neighbor TB Hamiltonian is modified by a phase factor, $H_i(k, \phi) = H_i^0(k) \exp(i2\pi \Lambda_i/\phi_0)$ (2)

where $\phi_0$ is the flux quantum and $\Lambda_i = \int_A \mathbf{A} \cdot d\mathbf{r}$. Analytically solving the Hamiltonian yields the electronic spectra of CNTs, $E(k, \phi)$, which can be used to further calculate the free energy of CNTs by using Fermi–Dirac function. Then, the orbital magnetic susceptibility can be obtained from the second derivative of free energy. This TB model reveals rich magnetic properties for CNTs: (1) Axial magnetic field induces periodic Aharonov-Bohm oscillations in CNT electronic structures, following a metal–insulator transition depending on tube diameter and chirality (Figure 7(a)–(c)). (2) A magnetic field perpendicular to the CNT axis does not change the bandgap, but can cause quantized Landau levels in...
the electronic spectra of CNTs. (3) Under an axial magnetic field, metallic CNTs are paramagnetic while semiconducting CNTs are diamagnetic (Figure 7(e)), whereas under the perpendicular magnetic fields all CNTs are diamagnetic; moreover, magnetic susceptibility linearly scales with the tube diameter. These theoretical results well support early transport measurements of CNTs, such as giant magnetoresistance and conductance oscillation under axial magnetic fields. In particular, the periodic magnetic flux modulation of the CNT bandgap has been unambiguously observed independently by Coskun et al. and Zaric et al. from different experimental groups. Note that the conductance oscillation is easier to be observed in MWCNTs, since the oscillating period is around several Tesla for a normal MWCNT with $D = 20$ nm. For a SWCNT with $D$ normally being approximately 2 nm, the corresponding period is up to $10^3$ Tesla, unattainable in current experiments. However, a beating phenomenon in Aharonov-Bohm type of interference was found to enable effective conductance modulations in SWCNTs under a much smaller magnetic field.

**Mechano-Electro-Magnetic Coupling Effect in Carbon Nanotubes**

The rich electromechanical and electromagnetic coupling behaviors raise an interesting question regarding how the CNT electronic states are coupled to both strains and magnetic fields. To clarify this issue, Zhang et al. developed a theory based on the TB model by taking into account the uniaxial and torsional strains and magnetic fields. The corresponding Hamiltonian becomes

$$H_j(k, \xi, \phi) = H_j^0(k) \tau_j \left( \exp[ik \cdot \Delta r_j] \right) \exp \left[ i(2\pi/\phi_0) \int_A \cdot dr \right]$$

Solving Equation 4, they found strong mechano-electro-magnetic coupling effect in SWCNTs. First, the critical magnetic field required for the metal-insulator transition in CNTs shows a linear yet chirality-dependent modulation with strains (Figure 7(d)). Second, the susceptibility displays strain-induced...
peaks, whose values and distributions rely on both the chirality and tube diameter; interestingly, a switch between paramagnetism and diamagnetism can be realized at certain strain values (Figure 7(e)). Similar analyses have also been carried out by Zhang et al., who studied the beating of Aharonov-Bohm interference in strained SWCNTs and found that the beating pseudoperiod can be modulated by strain, in a way sensitive to the CNT chirality. Nevertheless, owing to the challenge in concurrently applying strain and magnetic field to CNTs, very limited experimental progress is found in this aspect. Cai et al. measured magnetoresistance of SWCNT bundles under hydrostatic pressure up to 10 GPa and observed a pressure-induced transition in magnetoresistance from positive to negative under high applied fields, which should be the first evidence of mechano-electro-magnetic coupling effect in CNTs. Strain-tunable magnetic properties of CNTs could open a range of applications, such as pressoelectronic and magnetoelectronic devices.

**Contact Effects with Substrates and Electrodes**

While CNTs possess a number of exceptional properties in vacuum, the inclusion of CNTs into electronic devices requires integration with substrates, such as dielectric layers, gates and metal contacts. The CNTs can experience massive changes of their properties when put on substrates, posing uncertainty to the performance of CNT-based devices. On the other hand, integrating CNTs and substrates to form hybrid structures may provide properties complementary to those of components. It is thus of both fundamental and technological importance to understand modification of CNT properties by various substrates.

**Carbon Nanotube on Metals**

In most devices, CNTs need to form contacts with various metal surfaces, such as Pt, Au, Ca, Al and Cu. The properties of CNT devices are found to depend on the contact metals. For example, a semi-conducting CNT in field-effect transistors (FETs) exhibits \( n \)-type properties with Ca electrodes but \( p \)-type with Pd electrodes. Ballistic \( n \)-type CNT-based FETs have also been fabricated by contacting semiconducting SWCNTs using Sc or Y, which, combined with the ballistic \( p \)-type CNT FETs using Pd contacts, enable doping-free fabrication of CNT-based ballistic complementary metal-oxide semiconductor devices. The origin of the doping character of semiconducting SWNTs has been a subject of intensive debate, and several mechanisms have been proposed for the \( p \)-type conduction: (1) the doping directly by the contacts, which usually occurs for the metals with high work function, such as Pt; (2) the chemical doping by processing the CNTs in oxidizing acids; (3) the doping by adsorption of atmospheric oxygen. Any of these mechanisms can in principle influence the transistor performance. As for the contact itself, the design of high-performance CNT devices is contingent upon knowing the physics at metal–CNT interfaces, which correlates with the contact area, the metal work function, and the tube diameter and chirality. Theoretical analyses on this topic have revealed that the interface conductance scales with contact length, in agreement with an earlier experiment; and an armchair tube couples better than a zigzag tube to ordered Au/Ag contacts. The CNT diameter is another important factor. Both metallic and semiconducting SWCNTs have been demonstrated to form high-quality ohmic contact with Pt, Rh, Pt and Y when the tube diameter is larger than 1.6 nm. For CNTs with diameter smaller than 1.0 nm, ohmic contact proves to be difficult even for metallic CNTs, possibly because small CNTs tend to form stronger CNT-metal bonding that results in larger height of the tunnel barrier at the interfaces. Using large-scale Landauer transport calculations, Nemec et al. revealed that the superiority of Pd is correlated with the nature of CNT-metal interaction, manifested as weak hybridization with a large contact length. Further progress in this area calls for computationally more effective methods that could bridge the gap between experimental and theoretical scales of systems.

**Carbon Nanotube on Non-Metal Substrates**

The non-metal substrates include insulating and semiconducting substrates. Compared to metal substrates, the non-metal substrates often have less charge exchange with CNTs. On insulating substrates, such as SiO\(_2\) and h-BN, CNTs have little change in electronics, except for possible radial deformation induced by substrate adsorption. Some interesting behaviors can arise in CNTs adsorbed on semiconducting substrates, on which the electronic properties of CNTs are sensitive to local chemical environments. First-principles calculations showed that armchair CNTs can be chemisorbed on clean Si(001) via the formation of Si–C bonds, which enhance the metallic character of the nanotubes. In another work, the CNTs on Si(001) were shown to have different favorable adsorption sites depending on the nanotube directions and the local...
substrate geometry, entailing distinctly different electronic structures to the CNTs.\textsuperscript{110,111} Zigzag CNTs were also predicted to strongly adsorb on InAs, primarily by the hybridization between the carbon π orbitals and cation dangling-bonds of substrate; differently aligned CNTs on nonpolar InAs surfaces form almost the same band alignment while on polar surfaces the CNTs can be auto-doped into \( n \) or \( p \) type due to large surface dipoles,\textsuperscript{112} suggesting that CNTs can acquire richer functionalities on binary substrates. Integrating CNTs with semiconductor surfaces will inherit huge expertise from current semiconductor technology and will benefit the development of nanoscale hybrid electronic and optoelectronic devices.

**GRAPHENE-LIKE NANOSTRUCTURES**

**\( h \)-BN Nanostructures**

Monolayer h-BN sheet is an isostructural and isoelectronic analogue to graphene, and could serve as an excellent substrate for high-performance graphene electronics.\textsuperscript{113} Scalable growth of quality h-BN monolayers has been achieved through chemical vapor deposition on a range of substrates.\textsuperscript{114–116} The h-BN monolayer is featured by its bond ionicity, which localizes the electronic states and results in enhanced chemical and thermal stabilities. Thus, h-BN sheet shows unique potential of fabricating nanoscale devices operable in harsh environments. On the other hand, the bond ionicity breaks the symmetry of electronic states and opens a large bandgap near the Fermi level, rendering all h-BN nanostructures electronically insulating. The insulating properties severely hinder the applications of h-BN in functional devices. Extensive research efforts have been devoted to modifying the electronic properties of h-BN nanostructures, in particular those of nanotubes and nanoribbons.

**Boron Nitride Nanotubes**

BN nanotubes (BNNTs) are isostructural to CNTs.\textsuperscript{117,118} Mechanically, BNNTs possess excellent mechanical properties with a Young’s modulus up to 0.7 TPa\textsuperscript{119} as well as superb yield strength against axial tension.\textsuperscript{120,121} Electronically, the BNNTs remain insulating with a bandgap approximately 5.5 eV independent of the tube chirality, in contrast to CNTs. Another unique feature is that most BNNTs are in zigzag type because of the preference of aligning tube axes along the (1010) direction of h-BN during synthesis.\textsuperscript{122} When the tube diameter is less than 0.95 nm, strong rehybridization effect can rapidly reduce the bandgap of zigzag BNNTs with decreasing diameter.\textsuperscript{123} Moreover, zigzag BNNTs experience an axial deformation approximately 1% under an applied external electric field of 1 V/Å, attributed to both electrostrictive effect and converse piezoelectric effect, and the deformation ratio increases with decreasing tube diameter.\textsuperscript{124} In recent years, the interest of pushing BNNTs toward electronic applications has been boosted by a variety of methods of tuning their insulating bandgap. Mechanically, Kim et al., found that a radial deformation at a transverse pressure of about 10 GPa can decrease the bandgap of zigzag BNNTs down to 2 eV,\textsuperscript{125} due to the downshift of \( \pi^* \) states. Electrically, the bandgap of BNNTs can be significantly reduced by transverse electric fields\textsuperscript{126,127} and the gap modulation is more notable with increasing the tube diameter, showing a giant Stark effect as confirmed in subsequent experiment.\textsuperscript{128} The bandgap modulation in BNNTs by strain or electric field is superior to that by means of chemical routes, such as dopants\textsuperscript{129} or functionalizations,\textsuperscript{130} in a sense that the latter incurs localized states detrimental to device performance. Chemically, fluorination proves to be effective to enrich the functionalities of BNNTs, such as inducing \( p \)-type doping\textsuperscript{129} and long-ranged ferromagnetic spin ordering that is even tunable by radial deformation.\textsuperscript{131}

The experimentally synthesized BNNTs tend to be multiwalled, mostly even walls.\textsuperscript{132} The interwall interaction can significantly affect the electronic properties of multiwalled BNNTs. For example, the bandgap of a multiwalled BNNT is found to be remarkably narrower than any of its single-walled constituents; the valence band maximum (VBM) and conduction band minimum (CBM) are distributed on the outermost and innermost tubes, respectively.\textsuperscript{133} Thus, the multiwalled BNNTs can serve as a coaxial semiconductor junction with type II band alignment across the radial direction. Zhang et al. predicted that the band alignment between the inner and outer walls of a double-walled BNNT can be tuned from type II to type I by radial deformation, following a direct to indirect bandgap transition and a substantial gap reduction\textsuperscript{134}; moreover, the bandgap of a squashed double-walled BNNT can be further significantly reduced by a transverse electric field. Zhang et al. further showed that small double-walled BNNTs could be natural homogeneous nanocables as injected electrons prefer abnormally to concentrate on the inner wall while the outer wall keeps electrically neutral, breaking the tradition of heterogeneous coaxial structures for common cables.\textsuperscript{135}
BN Nanoribbons

BN nanoribbons (BNNRs) have also been the focus of much research attention (see Figure 8(a) and (b) for structures). BNNRs can be synthesized with high quality by longitudinally splitting of BNNTs or by morphology control of metal catalysts during chemical vapor deposition. The BNNRs with standard armchair (A-BNNRs) and zigzag edges (Z-BNNRs) are of particular interest. Without edge passivation, the A-BNNRs are nonmagnetic semiconductors while the Z-BNNRs have a magnetic ground state with extended spin ordering along the edges. With hydrogen passivation, all BNNRs become nonmagnetic insulators; the Z-BNNRs have decreased bandgap with increasing ribbon width due to enhanced transverse electric polarization. In the past few years, extensive theoretical efforts have been devoted to narrowing the bandgap of hydrogen-passivated BNNRs. Zhang et al. showed for the first time that the bandgap of BNNRs can be reduced by applying transverse electric fields, resulting in giant Stark effect due to reduced electric field screening; it is of practical importance that the gap modulation is more sensitive in a wider BNNR (Figure 8(c)-(d)). Later on, similar results were reported for large-width BNNRs by Louie et al. External electric fields could also couple with the spin ordering along the edges of bare BNNRs, giving rise to magnetic metal–semiconductor–half-metal transitions. However, the field strength required for desirable bandgap modulation

**FIGURE 8** Tunable electronic properties of BN nanoribbons. (a,b) Atomic structures of (a) zigzag and (b) armchair nanoribbons, with widths of $n_z = 8$ and $n_a = 15$, respectively. (c,d) Bandgap as a function of field strength for the (c) zigzag and (d) armchair nanoribbons. Dot lines in (c) are for the modulation under reversed electric field (pointing from the N edge to the B edge). (Reprinted with permission from Ref 4 Copyright 2008 American Physical Society). (e) Band structures and partial charge densities (0.006 e/Å$^3$) for the VBM (green) and CBM (violet) in aligned zigzag nanoribbons with different ribbon numbers. (Reprinted with permission from Ref 136 Copyright 2013 Royal Society of Chemistry).
reaches the level of V/nm, which remains too strong for practical application. Alternatively, introducing impurity states into the BNNRs by either chemical decoration at the edges or defect engineering proves to be an effective way. The Z-BNNRs can be functionalized into metallic, magnetic and even half-metallic materials by partial hydrogenation,\textsuperscript{141} or embedding line defects\textsuperscript{142,143} or edge attachment of oxygen or sulfur atoms.\textsuperscript{144} However, manufacturing these functionalized BNNRs still requires sophisticated fabrication processes which render the demand for mass production impractical. Also, the bandgap of both A- and Z-BNNRs can be effectively modulated by uniaxial strain.\textsuperscript{145,146} In particular, the spontaneous electric polarization in Z-BNNRs can strongly couple with the elastic strain, offering not only more sensitive strain modulation in a wider ribbon but also a novel piezoelectric behavior.

**Functional BN Nanostructures**

Given the experimental subtlety in realizing strong electric field and mechanical strain, a concept of intrinsic Stark effect induced by built-in electric polarization was demonstrated by Zhang et al. to spontaneously tune cubic BN nanofilms into semiconductor and even metal.\textsuperscript{147} Using hybrid DFT calculations with van der Waals correction, Zhang et al. further showed that polar BNNRs can be favorably aligned edge-by-edge via substantial hydrogen bonding at the interfaces,\textsuperscript{136} which induces significant interface polarizations and sharply reduces the bandgap of BNNRs well below silicon range (Figure 8(e)). Chemically, fluorination could transform a h-BN multilayer into a semiconducting c-BN nanofilm, which possesses substantial ferromagnetism upon electron doping.\textsuperscript{148} Substrates also modify the intrinsic properties of h-BN sheet in a significant way. It was predicted that an oxidized h-BN sheet supported on Cu substrate exhibits metallic properties when O adatoms vertically bond with B atoms.\textsuperscript{149} Further study showed that, upon chemisorption of ozone molecules or O-H groups on B atoms, the h-BN sheet on Cu exhibits ferromagnetic, antiferromagnetic or ferrimagnetic ordering depending on the adsorption density and configuration of functional groups.\textsuperscript{150}

**Metal Dichalcogenide Nanostructures**

As one of inorganic analogues of graphene, single-layer transition metal dichalcogenides (TMDs) MX\textsubscript{2} (M=Mo, W, Ta, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Nb; X=S, Se, Te) have sparked tremendous research interest as they can be superior to graphene in certain respects (also summarized in recent reviews\textsuperscript{151,152}). Of particular interest is the MoS\textsubscript{2} monolayer, in which one Mo layer is sandwiched between two S layers in a trigonal prismatic lattice (Figure 9(a)). The crystal field splitting of Mo d orbitals combined with reduced dimensionality yields a direct bandgap of 1.8 eV at the K point (Figure 9(d)),\textsuperscript{156} which is desirable for fabricating FETs, photo detectors, photonic devices. In contrast, few-layer and bulk MoS\textsubscript{2} have indirect bandgap, with the VBM at the \(\Gamma\) point and CBM at a point in the \(\Gamma-K\) path.\textsuperscript{157} The direct-indirect transition is believed to stem from the interlayer van der Waals interaction.\textsuperscript{156,158}

**In-Plane Strain Effect**

Electronic structures of monolayer or few-layer MoS\textsubscript{2} are very sensitive to elastic strains, which can be realized by putting MoS\textsubscript{2} samples on a flexible substrate and then deforming the substrates, or directly on a piezoelectric substrate (Figure 9(b) and (c)).\textsuperscript{153,154} Among different forms of strains, the biaxial strain is most effective for tuning the bandgap. For monolayer MoS\textsubscript{2}, DFT studies showed that a direct-to-indirect bandgap transition can occur at a biaxial tensile strain of approximately 1\% (Figure 9(e)), as a result of the downshift of the topmost valence band at the K point with respect to that at the \(\Gamma\) point.\textsuperscript{153,159} Meanwhile, as shown in Figure 9(e), both the direct gap at the K point and the indirect bandgap between the K and \(\Gamma\) points are reduced, caused by the rapid downshift of the CBM. Further, the monolayer MoS\textsubscript{2} can become metallic at a biaxial tensile strain over 10\% or compressive strain over 15\%.\textsuperscript{160} Tensile strain could also enhance the carrier mobility in monolayer MoS\textsubscript{2} by increasing the band dispersion. Applied uniaxial tensile and shear strains also dramatically reduce the bandgap of monolayer MoS\textsubscript{2}.\textsuperscript{161} For few-layer MoS\textsubscript{2}, photoluminescence spectra revealed that the bandgap decreases by 120 meV per 1\% uniaxial tensile strain in bilayer MoS\textsubscript{2}\textsuperscript{153} and increases by approximately 300 meV per 1\% biaxial compressive strain in trilayer MoS\textsubscript{2}.\textsuperscript{154} It appears that the strain-tunable bandgap is more sensitive in thicker MoS\textsubscript{2} layers, thanks to the coupled effect of the in-plane strain and the out-of-plane deformation due to the Poisson effect. Moreover, biaxial compressive strain causes a significant increase of photoluminescence intensity in trilayer MoS\textsubscript{2}.\textsuperscript{154}

**Out-of-Plane Strain Effect**

We now discuss the effect of out-of-plane strain. Dou et al. detected that under hydrostatic pressure the optical transition of a bilayer MoS\textsubscript{2} changes from
direct ($K-K$) to indirect ($\Lambda-K$), due to a changeover of the CBM from the $K$ point to the $\Lambda$ point. Peña-Álvarez observed that under vertical compression the monolayer MoS$_2$ experiences a direct-to-indirect gap transition at 0.5 GPa and ends up with semimetal at 3 GPa. Hydrostatic pressure could also induce a semiconductor–metal transition in multilayer MoS$_2$ due to an overlap of valence and conduction bands as the interlayer distance decreases. In contrast, Tongay et al. found that the interlayer interactions in few-layer MoSe$_2$ can be weakened by thermal expansion, which leads the system properties close to the limit of monolayer.

**Magnetic 2D TMDs**

As mentioned, 2D TMDs can also exist as MX$_2$ with $M=$Sc, Ti, V, Cr, Mn, Fe, Ni, Nb, W, Ta, Sn and X=S, Se. These TMDs have lattice structures similar to MoS$_2$. Specifically, the CrS$_2$, CrSe$_2$, FeS$_2$, FeSe$_2$, MoS$_2$, MoSe$_2$, WS$_2$, WSe$_2$, TaS$_2$ and TaSe$_2$ energetically favor the 2H phase, while TiS$_2$, TiSe$_2$, MnS$_2$, MnSe$_2$, NbS$_2$, SnS$_2$, and SnSe$_2$ favorably adopt the 1-T phase (see Figure 9(a), right); whereas the ScS$_2$, ScSe$_2$, VS$_2$, VSe$_2$, CoS$_2$, CoSe$_2$, NiS$_2$, NiSe$_2$ and NbSe$_2$ can be stable in both phases with competitive stability. The subgroup of 2D MX$_2$ with $M=$Mo, W and $X=$S, Se are very similar to the 2D MoS$_2$ in terms of lattice and electronic structures; the rest can exhibit distinct properties, such as magnetism. Straining 2D magnetic TMD monolayers could weaken the metal-ligand bonding and localize metallic electronic states therein. This will change the exchange interaction between local spin moments and result in remarkable mechano-magnetic coupling. *Ab initio* study showed that the magnetism in the 2D VSe$_2$ monolayer can be enhanced by applying a biaxial tensile strain, and the ferromagnetic ordering is robust against deformation. In contrast, the ground state of 2D NbSe$_2$ can be switched from antiferromagnetic to ferromagnetic when a biaxial...
tensile strain over 4% is applied as energetically reflected in Figure 10 by energy. Also, a biaxial strain over 6% switches the ground state of 2D TaS$_2$ and TaSe$_2$ from Pauli-paramagnetic to ferromagnetic. Both SnSe$_2$ and SnS$_2$ monolayers are semiconducting with indirect bandgaps, which can be closed under an applied biaxial strain of approximately 10%.

Currently, experimental progress of fabricating the 2D TMDs is advancing rapidly, and the syntheses of 2D WS$_2$, WSe$_2$, VS$_2$, NbSe$_2$, NbS$_2$, VSe$_2$, and NiTe$_2$ have been reported successively. Unfortunately, the reports of magnetism in these 2D TMDs are very few, possibly because the synthesized samples are not sufficiently thin. So far, only the ultrathin VS$_2$ nanosheets was reported to be ferromagnetic by Gao et al., and all other magnetic 2D TMDs remain to be confirmed by dedicated experiments.

Phosphorene Nanostructures
Phosphorene, a monolayer of black phosphorus, has been a rising star material since the first demonstration of using it for fabricating high performance FETs. In contrast to the honeycomb lattice of graphene, h-BN and TMDs, the lower-symmetry puckered structure of phosphorene (Figure 11(a)) leads to superior mechanical flexibility and anisotropic electronics. The band structure of phosphorene shows direction-dependent dispersion near the Fermi level (Figure 11(b)), giving rise to anisotropic electric conductance and carrier mobility.

Structural flexibility of phosphorene offers a great opportunity to tune its electronic properties by elastic strain. Theoretically, a single-layer phosphorene can withstand a tensile stress and strain up to 10 N/m and 30%, respectively. The electronic states near the band gap show different distributions in their wave function, so that they respond differently to strain (Figure 11(b)), leading to an effective modulation of the conductance anisotropy. For instance, a moderate biaxial or uniaxial strain causes a 90° rotation of the preferred conducting direction, as supported by the change of electron effective mass shown in Figure 11(c), which is attributed to the changeover of the lowest conduction bands with different anisotropic dispersions (Figure 11(b)). Regarding the bandgap, biaxial compressive strain decreases the gap value and induces a semiconductor–metal transition at −9% strain; whereas biaxial tensile strain first increases the gap to a peak at 4% strain and decreases it thereafter (Figure 11(d)), just as a result of the preceding changeover of the lowest conduction band at 4% strain. Upon applying a uniaxial strain, the bandgap...
of phosphorene can experience a direct–indirect–
direct transition; moreover, the conduction band
extreme converges at some critical strain, yielding
enhanced thermoelectric performance.\textsuperscript{184}

In addition to strain, external electric
fields have also been adopted to tune the electronic proper-
ties of phosphorene. A recent theoretical study
revealed a Stark effect in phosphorene under electric
fields applied along the normal of the basal plane,
showing continuous gap modulation.\textsuperscript{179} In few-layer
phosphorene, applied vertical electric field leads to
even richer functionalities as increasing
field strength not only decreases the bandgap but induces a transi-
tion from normal insulator to topological insulator
and finally to metal.\textsuperscript{185}

Research attention has also been paid to phos-
phorene nanoribbons, nanotubes and van der Waals
multilayers. Both armchair and zigzag phosphorene
nanoribbons with H-passivated edges inherit the semi-
conducting nature of phosphorene, and their bandgaps depend on the ribbon width $w$.\textsuperscript{186} The bandgap of the armchair phosphorene nanoribbon scales as $1/w^2$, while that of the zigzag phosphorene nanoribbon exhibits a $1/w^2$ behavior.\textsuperscript{187} As for the multilayers, bilayer phosphorene under a small verti-
cal compression exhibits a high electron mobility of $7 \times 10^4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at room temperature as a result
of a newly emerged conduction band extreme.\textsuperscript{188}

Other Newly Emerged 2D Material
and Related Nanostructures

All above 2D materials are naturally lamellar in their
bulk forms, with the component layers assembled by
van der Waals interaction. Recently, the research
enthusiasm on 2D materials has been extended to
those, whose bulk forms are not layered in nature.
These 2D materials include hexagonal MXenes, sili-
cene, germanene, ZnO sheets and tetragonal TiC
monolayer, etc, which need special conditions for sta-
bilization, such as structural buckling, chemical pas-
sivation and support on substrates.

**MXenes**

MXenes can be obtained by etching out the A layers
from MAX materials at room temperature, where M is
an early transition metal, A can be a group IIIA or
IVA element, X is C and/or N.\textsuperscript{189} The MXene family

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure11}
\caption{Geometry structure and intrinsic anisotropy of phosphorene. (a) Atomic structure in the top and side views. (b) Band structures of monolayer phosphorene under (left) 0 and (right) 5% biaxial tensile strains, where the bands along the $\Gamma$-X and $\Gamma$-Y directions have anisotropic dispersion. (c) Direction-dependent electron effective mass of phosphorene under (left) 0 and (right) 5% biaxial tensile strains. (Reprinted with permission from Ref 178 Copyright 2014 American Chemical Society) (d) Bandgap and strain energy $\Delta E$ of phosphorene as functions of the biaxial strain. (Reprinted with permission from Ref 179 Copyright 2014 American Chemical Society).}
\end{figure}
includes 2D Ti$_2$C (Figure 12(a)), Ti$_3$C$_2$ (Figure 12 (b)), Nb$_2$C, V$_2$C, (Ti$_{0.5}$Nb$_{0.5}$)$_2$C, (V$_{0.5}$Cr$_{0.5}$)$_3$C$_2$, Ti$_3$CN and Ta$_4$C$_3$. All bare MXene monolayers are terminated by M layers and therefore are strongly metallic, with a high electron density of states near the Fermi level. Chemical passivation of MXene surfaces eliminates the metallic states and results in 2D semiconductors and even topological insulator. Very recently, the 2D Sc$_2$CF$_2$ is fabricated and used to construct vdW heterostructures with the MoS$_2$ monolayer, whose electronic structure turns out to be extremely sensitive to in-plane biaxial strain: a 1.5% tensile strain suffices to induce an insulator-metal transition. While most MXenes are non-magnetic, the 2D Cr$_2$C, Cr$_2$N, or Ta$_3$C$_2$ are ferromagnetic and the 2D Ti$_3$C$_2$ and Ti$_3$N$_2$ are antiferromagnetic (Figure 12 (c)). Like magnetic TMDs, these MXenes have tunable magnetism by in-plane strain as well. The intrinsic magnetic moments of 2D Ti$_2$C and Zr$_2$C are 1.92 and 1.25 $\mu$B per primitive cell, which can be enhanced by 11.5 and 60% under biaxial tensile strains of 8 and 3%, respectively. For 2D M$_2$C (M=Hf, Nb, Sc, Ta, V), their nonmagnetic ground state can be switched to ferromagnetic one by tensile strain, with the critical strain for the switch depending on M. These results, together with those of magnetic 2D TMDs, feature a universal behavior of tailoring the magnetism of 2D materials by engineering strain.

**Silicene and Silicene-Like 2D Materials**

Silicene (Figure 12(d)), germanene, arsenene (Figure 12(e)) and antimonene are a group of 2D materials with honeycomb lattice yet out-of-plane structural buckling. Silicene, the silicon analogue of graphene, is a gapless semimetal with a Dirac cone in its band dispersion and can open a bandgap that is linearly tunable by an applied vertical electric field. While the synthesis of silicene has been reported for several years, its transfer from catalytic metal substrates for fabricating FETs was demonstrated until recently.
In contrast, arsenene and antimonene are semiconductors with indirect bandgaps of 2.49 and 2.28 eV, respectively. Applied tensile strain can sensitively modulate the bandgaps of arsenene and antimonene from indirect to direct, accompanying with a substantial bandgap reduction in the arsenene.

**2D ZnO Monolayer**

When a ZnO (0001) nanofilm is only a few ZnO layers thin, it prefers a planar configuration, like the h-BN sheet, driven by the disappeared surface dipole. A monolayer of such ZnO sheet can be shaped into nanoribbons, whose electronic properties are unusual due to peculiar edge states and are tunable by external electric fields and edge passivations with hydrogen. In particular, bare zigzag ZnO nanoribbons exhibit edge magnetism that can be remarkably modulated and even completely quenched by applied transverse fields, depending on the field direction.

Beyond the hexagonal 2D materials, Zhang et al. predicted a 2D tetragonal TiC (Figure 12(f)) monolayer sheet with zigzag-shaped buckling structure, which possesses anisotropic electronic properties and an indirect bandgap of 0.21 eV, thus promising for applications in nanoelectronics.

**CONCLUDING REMARKS**

We have comprehensively reviewed the progress on tunable electronic and magnetic properties of low-dimensional materials, with focus on the modulation by external electric field, strain and substrates. In spite of the significant difficulties in applying the electric fields and nanoscale strain and in performing related analyses and characterizations, notable breakthroughs in realization of tunable properties in different low-dimensional materials have recently been achieved within several experimental groups. Fully delivering these useful properties into applications remains contingent upon the development of advanced fabrication technology, especially the ability to reliably and repeatedly handle the modulation.

On the theoretical side, the main challenge is to develop new and/or optimize existing and promising principles governing the tunable properties as well as to demonstrate their transferability and sometimes preferable applications when integrating the nanomaterials into a device system. For example, for one-dimensional layered materials, applied electric field vertical to the basal plane is more compatible with current device basis than the transverse fields, as recently demonstrated for realizing half-metal in GNRs. Moreover, instead of applying strong external electric fields, using the built-in electric fields in materials or at the interfaces is another direction deserving further attention; yet how the built-in electric fields can be effectively manipulated remains an open question. On the other hand, to take full advantage of the strain effect in low-dimensional materials, it is important to explore innovative technologies that can enhance the strain sensitivity and that enable the operation of strain in a cost-effective and technically feasible way. Moreover, whether there is a theory capable of describing the nanoscale strain–functionality relationship, just as an extended version of conventional strain–stress relationship in continuum, is also an appealing question.

Aside from the mechano-electro-magnetic coupling, the coupling effects induced by various fields in low-dimensional materials can be extended into a broader spectrum, which includes opto-electronic, magneto-optical, thermo-optical and photo-acoustic couplings etc. Having all the atoms exposed on the surfaces, the low-dimensional materials have become an important platform for exploring these peculiar couplings with high sensitivity and efficiency toward manipulating their intrinsic properties and developing novel applications. For example, the two-dimensional MoS$_2$ monolayer, with inherent spin–orbit coupling and inversion symmetry, has the valley and spin inherently coupled to enable control of valley polarization by optical pumping with circularly polarized light, which opens the door for developing integrated valleytronic and spintronic applications. While detailed discussion of these aspects is beyond the focus of this report, they are all promising research directions for realizing the full potential of low-dimensional materials.

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