2D Materials: Future and Perspectives

Abstract

The physics of two dimensional (2D) materials is always intriguing in their own right. For all of these elemental 2D materials, a generic characteristic feature is that all the atoms of the materials are exposed on the surface, and thus it turns out to be comparatively easier to tune the structure and physical properties of the materials by surface treatments. The discovery of graphene have fostered an intensive research interest in the field of graphene like 2D materials such as silicene, germanene (hexagonal network of silicon and germanium respectively), stanene, borophene etc. really a zoo of 2D materials.

Mini Review

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Introduction

2D Materials are commonly defined as crystalline materials consisting of a single layer of atoms. Most often, it is classified as either 2D allotropes of various elements or compounds consisting of two or more covalently/ionically bonding elements. In these layered structured materials, the atomic organization and bond strength along two-dimensions are similar as well as quite stronger than along a third dimension where they are bonded together by weak 'van der waals' interaction [1,2]. In nature, the organisation of nanofibers on the feet of geckos increases sufficiently the surface area of their feet so that they can easily walk upside down even on a slippery surface. It is interesting to note that carbon nanotubes first discovered by Iijima [3] were the rest isolated 2D materials. In Figure 1, we show some of the important members of this 2D family. The recent developments of two-dimensional (2D) materials have fostered a great deal of research interest since the first isolation of graphene [4-12]. The emergence of each new material brings excitement as well as puzzles in their characterization and physical properties. These 2D materials offer an un-usual platform for predicting various heterostructures suitable for versatile applications.

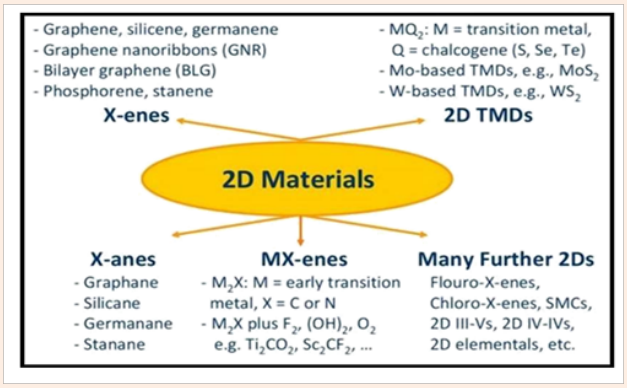

Figure 1: An incomplete zoo of 2D materials.

The properties of these materials are usually distinctly different from those of their 3D counterparts. Besides, these characteristic 2D materials offer reasonable flexibility in terms of tailoring their electronic properties. Apart from that, there are indeed a class of new novel Dirac materials [13,15] and heterostructures in 2D available either theoretically or experimentally to verify some basic physics along with fabrication of nanodevices. In Figure 2, we schematically present some of the materials possessing Dirac cones. Transition-metal dichalcogenides (TMDCs), another important key member of 2D family also have high potential in device application from the point of view of thin film [16]. It is highly encouraging that most of the 2D materials isolated so far are able to cover the entire range of the electromagnetic spectrum.

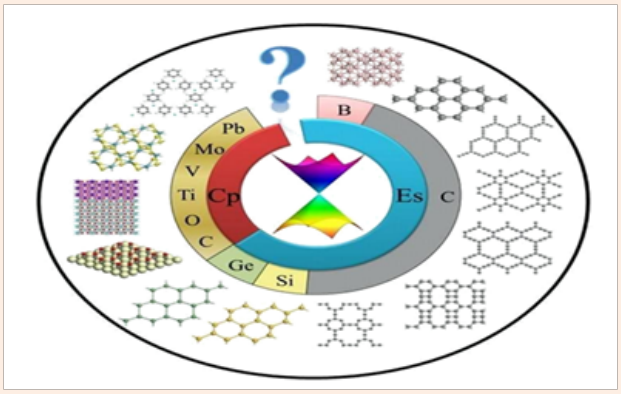

Figure 2: 2D materials with Dirac cones consisting of various elements and compounds. Reproduced from [15].

It is quite understandable that the experimental studies often take sufficient time as well as resources to predict and control the physical properties of 2D materials. On the other hand, with the help of minimal resources, the computational study, in particular the first-principles calculations [14], (apart from the stability of the proposed 2d structures) have taken a key role in engineering the band gap, scanning tunneling microscopy (STM) images, optical and magnetic properties. It will be important to compare [3] the predicted numerical results thus obtained from the density functional theory (DFT) to the experimental one.

The most important of all these materials is the value of the band gap which can be further tailored by applying in plane stress, an external electric field, chemical functionalization and defects. For example, band gap opening in graphene is site specie for boron (B) and nitrogen (N) doping [17]. Even the optical properties are significantly modified [18,19] by B and N doping. N-B co-doping can enhance the static dielectric constant. Electronic density of states can be modified by the presence of disordered Stone-Wales defects in graphene [20]. Transition metal (TM) specially titanium at hollow site (Ti@HS)) can influence [21] significantly the optical properties in compared to pristine graphene. Besides, when the distance between two bilayers of graphene is greater than 5Å, then the system is equivalent to single layer [22]. On the other side, a theoretically proposed tetragonal graphene (T-graphene) also shows some interesting features in their electronic and optical properties [23-25]. Higher stability, large dipole moment along with high intensity Raman active modes are observed in N-doped T-graphene [26]. In Figure 3, some of the allotropes of graphene proposed so far have been depicted. Even the size and morphology of graphene quantum dot can influence the electronic and optical properties [27]. In particular, graphene plasmonics has been a rapidly emerging area for fast tunable lighting at the nanoscale [28]. Graphene and MoS_2 have been routinely used in surface-enhanced Raman spectroscopy (SERS) applications [29]. Besides, inorganic 2D materials have shown improved performance in lithium and sodium batteries [30].

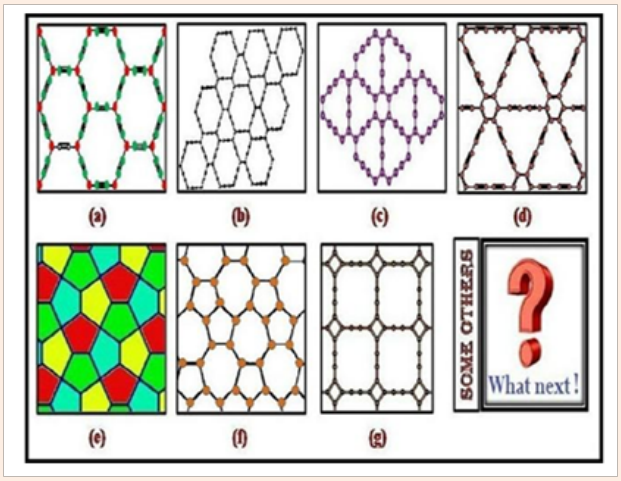

Figure 3: Graphene allotropes (a) ∝ graphyne (b) β graphyne (c) ϒ graphyne (d) graphdiyne (e) penta-graphene (f) pentaheptites (g) R-graphene [23].

Buckled 2D-Xenes (X = Si, Ge, Sn and so on) sheets have shown varied novel electronic structure ranging from trivial insulators, to semiconductors with tunable gaps, to semi-metallic, depending on the substrate and topological insulator [31,32]. Silicene, the first member in the 2D-Xenes family [33-38] beyond graphene reserves its own place. The magnetic properties can be tailored by chemical functionalization, such as hydrogenation and introducing vacancy into the pristine planar silicene [39] and silicene/graphene hybrid [40]. The importance of shape dependence and optical anisotropy properties in silicene nanodisks establishes that a zigzag trigonal (ZT) possesses the maximum magnetic moment [41]. Besides, diamond shaped (DS) silicene nanodisk shows the highest static dielectric constant [41] having no zero energy states [42]. Further, the optical properties of planar silicene can be significantly influenced [43] by phosphorous (P) and aluminum (Al) in the silicene network.

Germanene, third member of these 2D family places its impression due to its high spin-orbit coupling and its properties has been compared with silicene and graphene both experimentally and theoretically [23,44-46]. The site dependent adatoms arsenic and gallium [47] and beryllium [48] in the germanene network can significantly modify the electronic and optical properties. Aluminene, 2D allotrope of aluminium has been demonstrated as highly whole doped graphene [49]. In recent years, borophene [50,51] and stanene [52,53] have been emerged as promising 2D materials for device application.

These 2D materials being ultra-thin possess high degree of anisotropy and chemical functionality. They are highly diverse in character in size, morphology along with biocompatibility and degradability. Because of these essential properties, scientists have been highly motivated to use these novel and emerging robust 2D materials in drug delivery systems, imaging, tissue engineering, and biosensors [54]. They are probing the possibility to tailor the physiological interactions of biomedical nanocomposites with living tissues. In fact, the complexities involved in variable particle size and shape, impurities from manufacturing hold the essential key in this research.

Conclusion

To conclude, the unconventional and multi-functional features associated with these novel 2D materials will trigger further research and will hopefully overcome the constraints appeared along with for the nano-device application. Thus, at this stage of research, it is highly desirable that further experimental investigations should be pursued for bulk manufacturing of pure and defect free 2D materials at a reasonable economical price with a suitable band gap required for functioning in a chip. In this regard, the powerful theoretical predictions from various DFT computations of 2D materials with proper electrical composites might be helpful to design the pavements for devices. In fact, this is indeed the right time to look for novel heterostructures beyond graphene for fabricating faster, smaller and smart nanoelectronics devices required essentially for the next generation.

Acknowledgment

None.

Conflicts of Interest

None.

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