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Future Prospect of Plumbene: A Review

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Abstract: Discovery of graphene and its bewildering properties have brought forth another class of materials known as "two dimensional materials" or 2D materials. Spurred by the achievement of graphene, alternative layered and non-layered two dimensional materials have become the focal point of extraordinary research because of their novel physical and chemical properties. Plumbene, a single layer of lead (Pb) is the latest two dimensional material, has pulled in huge enthusiasm inferable from its uncommon properties and possible applications. In this paper, we investigation about the most recent advancement in the investigation of Plumbene, for the most part on the structure, growth techniques, physical properties, future applications and difficulties. The phenomenal mechanical and thermal properties of Plumbene will open the best approach to batteries, machine manufacturing, shipbuilding, etc. Lastly, this review concludes with a future forthcoming to manage this quick advancing class of two dimensional materials in cutting edge materials science.

Keywords: Two-Dimensional layered materials; Plumbene; Topological Insulators; Spintronics

1. Introduction

The commendable achievement of graphene¹⁻⁴), that's few of the firsts of these two-dimensional (2D) materials has started a runaway impact in the quest for examining other 2D materials⁵). After the discovery of graphene, numerous researchers would not realize that a dozen 2D materials such as silicene⁶⁻⁸), germanene⁹⁻¹¹), and phosphorene¹²⁻¹⁶) and stanene¹⁷⁻²¹) etc. can be isolated and studied in the past two decades. The latest 2D material in this series is Group 14 element i.e. Plumbene²²), a monolayer of lead, having honeycomb structure is added. The chemical symbol of Lead is Pb, originating from the Latin word "plumbum" for lead; in this manner, a monolayer of the Pb film can be called "plumbene," in similarity with graphene and silicene. As the primary individual from the 2D family; the utilization of graphene has advancement over an expanded division of uses going from unconventional electronics gadgets²³) to biomedicine²⁴⁻²⁷) because of its exceptional properties, for example, ultra-high carrier mobility²⁸), ultra-low weight²⁹), high thermal conductivity³⁰), high optical transparency³¹), flexibility³²) and remarkable high strength³³). Regardless, graphene has tunable intriguing electronic properties³⁴), the spin-orbit (SO)³⁵⁻³⁶) coupling is feeble restricting its uses as spin filters³⁷), topological insulators (TIs)³⁸) and so forth. In this way, there is a critical demand to find novel

2D materials in after graphene to beat its lacks.

Topological insulators³⁹⁻⁴⁰) due to their nature, enforce the electrons to move on the surface at very high speeds subsequently concluding valuable uses in electronics and photonic devices. Investigation of the group 14 elements⁴¹), utilizing first-principles computations has uncovered enormous interest because it has the highest spin-orbit interaction, because of orbital electron structure of lead and consequently the highest energy band gap, which makes it a robust 2D topological insulator wherein the Quantum Spin Hall Effect⁴²) may arise even above room temperature.

2. Crystal Structure

The information about the stability of crystal structure and surface properties are basis for any 2D material if it is to have feasible utilization in any area of interest. This segment presents an understanding of the fundamental crystal arrangement of elemental structures.

In the different investigations related to the structure of Group IV components (C, Si, Ge, Sn and Pb)⁴³), it was proposed that the atomic arrangement of planar Group IV elements follow the hexagonal honeycomb structure of graphene⁴⁴⁻⁴⁵). Plumbene moreover has buckled honeycomb structure similar to graphene and silicene. Figure. 1a outlines the hexagonal structure and the

buckled nature of plumbene. The lattice constant of plumbene is recorded as 4.93 \AA^{22} , and buckling height (δ) is estimated between 0.97 \AA to 1.01 \AA^{46} . The Pb–Pb bond distance (d) i.e the nearest neighbour atoms in plumbene is 3.00 \AA^{22} , calculated by utilizing structural optimization. The bond angle between Pb–Pb atoms in plumbene is 108.34°^{22} which outcomes in buckled structure of plumbene. Overlapping between π – π bonds are additionally determined in plumbene analogous to graphene however weaker in nature than graphene due to longer bond length. In plumbene, due to its buckled configuration, overlapping between π and σ orbitals is higher, and accordingly the system is stabilized⁴⁶. A high band gap ($\sim 0.4 \text{ eV}$)⁴⁷ which is lots large than that of other group-IV 2D materials is detected in plumbene and subsequently can be a perfect material for a topological insulator.

It can furthermore have uses related to machine manufacturing, shipbuilding, and in batteries etc., wherein convectional lead is utilized so far. large band gaps are anticipated in decorated plumbene⁴⁸, which might lead to a quantum spin hall insulator⁴⁹ behaviour and captivating high-temperature applications. Certainly, synthesizing such sheets whereas maintaining their non-trivial properties remains a difficult task.

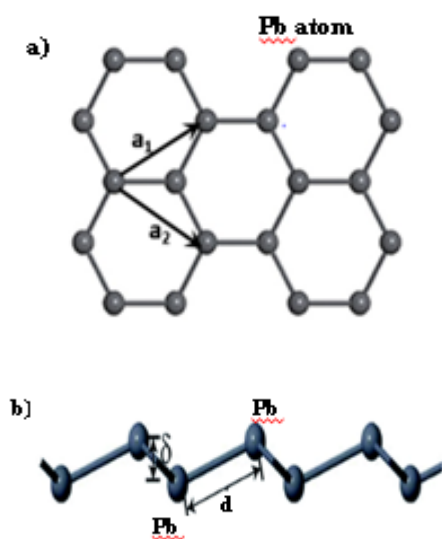


Figure. 1:(a) Top and (b) side view of honeycomb structure of plumbene, where a_1 and a_2 are the primitive vectors, δ is buckling height and d is the distance between Pb-Pb bonds.

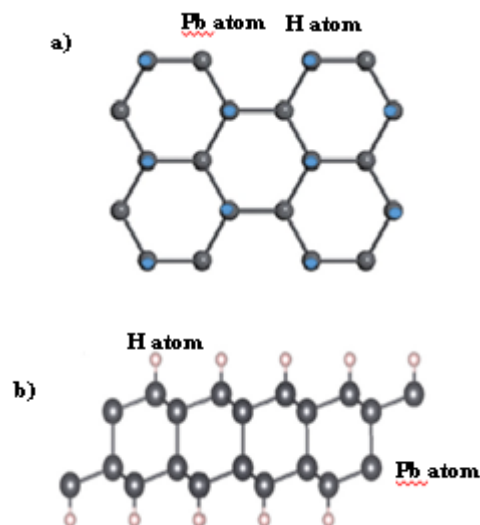


Figure. 2: (a) Top and (b) side view of the bilayer plumbene with Pb and H atoms, respectively.

The structure of different two dimensional group IVA materials with chemical functionalization have moreover been considered broadly, and a few with huge bulk gaps have been anticipated theoretically⁵⁰⁻⁵⁴. Moving from graphene to plumbene, the buckling height is found to be extended and the increase in atomic mass also prompts to a considerable rise in the effective spin orbit coupling (SOC)⁵⁵. It is notable that SOC assumes a significant part in quantum spin hall (QSH) insulators. Recently, A special class of 2D QSH insulators in X-decorated plumbene monolayers (PBX; X = H, F, Cl, Br, I) with unusually enormous bulk gaps from 1.03 eV to most elevated estimation of 1.34 eV has been predicted⁴⁷. Figure. 2 illustrates the structure of the bilayer plumbene, in which all adjacent Pb atoms are sp^3 hybridized. Remarkably, the optimized buckled height (δ) is found 0.82 \AA^{49} comparative to the case (0.78 \AA)⁴⁷ of monolayer plumbene. Also, a new family of methyl and trihalogenomethyl decorated plumbene monolayer⁴⁸ i.e. monolayer with $-CX_3$ where, X = H, F, Cl is investigated and report exceptionally huge band gaps within the range of 0.84 eV to 0.98 eV with spin-orbit coupling. These range of band gaps is considerable higher in comparison to many existing topological insulators and feasible at room temperature.

3. Fabrication Process

After the synthesis and characterization of graphene, there are various two dimensional materials which have been arduously examined with the objective of applying unique promising 2D material's properties^{3, 7, 8, 19-20}. After the revolutionary growth of silicene on Ag (111)⁸, the, down the column, group 14 mono elemental two dimensional honeycomb lattices were at the core interest. Before long, germanene and stanene, as well as silicene over again, have been acknowledged on different surfaces.

In addition, group 13 and 15 analogous such as borophene⁵⁶⁻⁵⁸, phosphorene⁵⁹, antimonene⁶⁰, and bismuthene⁶¹, have been synthesized too. The acknowledgement of the remaining material in the group 14 elements, i.e., plumbene, persisted a pursuit for the ambrosia, in spite of the fact that numerous hypothetical research forecast its stability and expected extraordinary intriguing properties.

In recent times, the synthesis of large area plumbene sheets were reported by Yuhara and co-workers⁶². The synthesis has been carried out by the epitaxial growth of plumbene by way of segregation from prepared $\text{Pd}_{1-x}\text{Pb}_x$ (111) alloys grown on Pd (111) substrates upon heating/alloying Pb thin films deposited⁶² at room temperature (Refer Figure. 3). The establishment and structure of plumbene sheets so acquired used to be examined via the usage of low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) which approves that a Pb sheet overlays the $\text{Pd}_{1-x}\text{Pb}_x$ (111) alloy and exhibit a planar honeycomb structure with a unit cell in accordance to that of freestanding plumbene.

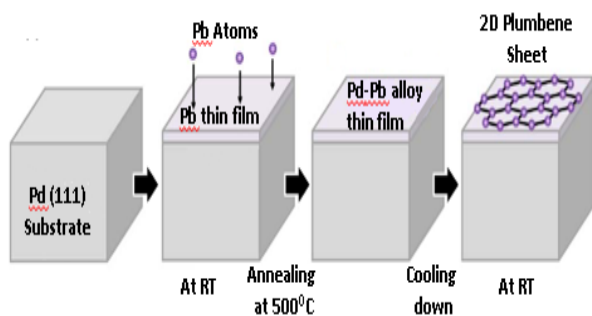


Figure. 3: Epitaxial growth of 2D honeycomb plumbene sheets⁶².

4. Properties of plumbene

This segment presents the progressing status on the comprehension of physical, electronic and magnetic properties of plumbene. The band gap in plumbene is much higher than other existing 2D materials such as graphene and silicene⁴⁷. Consequently, they are able to have possible applications including topological insulators and high-temperature operations. Structural configurations moreover bring about beneficial irreplaceable properties of plumbene than other two dimensional materials. Indeed, surprisingly it has prevalent properties in comparison to lead which can be used for the utility in batteries, machine manufacturing, shipbuilding, and so on, wherein traditional lead is utilized so far. Plumbene can too utilized for power generations, preparation of plumbene-reinforced nanocomposites, etc. Plumbene will have anticipated uses wherein conductivity is the major issue. Plumbene's thermal and mechanical properties are additionally described recently.

4.1 Electronic and topological properties

Topological insulators (TIs)^{38-39, 42}, also known as quantum spin hall (QSH) insulators³⁹⁻⁴⁰, as a novel class of quantum materials⁵⁵ have caused exhaustive investigation in quantum information, as they provide an unconventional and strong ground for attaining relativistic and spin-polarized Fermions in the condensed matter system.

As of now, two dimensional materials in groups IV and V are favourable applicant for the quantum spin hall effect characterized by using an insulating bulk-gap and gapless edge states at its boundaries due to time-reversal symmetry (TRS)⁵⁵, hence giving the alluring ideas to unique quantum electronic devices with low energy dissipation. Earlier studies have proved that 2D group IV elements, such as graphene^{63,64}, silicene^{65,66}, germanene^{67, 68}, and stanene^{69,70} are topological insulators⁵⁵ but plumbene is considered as a normal band insulator due to excessive strong SOC effect²².

Theoretical calculations foresee that a giant bulk gap can be acquired via fluorination, hydrogenation, or different sorts of functionalizations^{47,48}. Absorption of atom or molecule is required to saturate the p_z orbital or dangling bond so that a band gap can be released at the Dirac point except SOC. At the point, when the SOC is thought of, a larger gap can be acquired in the corresponding system. For instance, first-principles calculations forecast a 2D QSH insulator in F-decorated plumbene monolayer with an exceptionally large bulk gap of 1.34 eV⁴⁷⁻⁴⁹.

First-principles and tight-binding computation are used to explore plumbene's band structures and topological properties²². Results show that the system can change from a normal insulator to topological insulator with change in large bulk gap of ~ 400 meV to ~ 200 meV²². The QSH state is exceptionally strong with regard to external strain. Due to plumbene's simple structure, and external field effects on two large bulk gaps, it can be a favourable ground for topological phenomena and novel quantum device uses at room temperature.

Additionally, 2D materials with coexisting topological and ferroelectric ordering have been the centre of 2D condensed matter physics in late years, and their concurrence in a single system may make vital undiscovered development and potential uses. Recently, a class of ferroelectric topological insulators (FETIs) in CH_2OCH_3 -functionalized plumbene ($\text{Pb-CH}_2\text{OCH}_3$)⁷¹ is illustrated on the basis of first-principles calculations, which confirms the huge nontrivial band gap of 0.80 eV in $\text{Pb-CH}_2\text{OCH}_3$, made acquainted by the orbital filtering effect in the existence of spin-orbit coupling (SOC). These outcomes at the aggregate of topological and ferroelectric characteristics may give a new platform for the advancement of microelectronic devices and the use of spintronics at room temperature. Recently, plumbene on Fe layer has been explained theoretically. Fe layer being a ferromagnetic element prompts a noteworthy exchange

splitting in plumbene due to which, there is a transition from quantum spin Hall to quantum anomalous Hall state⁷²).

4.2 Magnetic Properties

It has been appeared that the 2D semiconductors combining with magnetic data storage materials might prompt to 2D spintronics devices with huge applications⁷³. The magnetic properties of 2D materials may be altered with the aid of using doping process or making adsorption of transition metal elements that could result in dilute magnetic semiconductors in 2D semiconductors⁷⁴.

To investigate the magnetism in plumbene, 3d transition metal elements such as Ti, V, Cr, Mn, Fe, and Co are doped in plumbene⁷⁵ which shows magnetic states in monolayer plumbene. All the computation have been accomplished the use of spin polarized density functional theory (DFT) including SOC, and Vienna ab initio simulation package (VASP). It was also observed that Sc and Ni-doped plumbene systems do not show magnetic solutions. The values of spin magnetic moments vary from 1.32 μ_B (minimum) to 4.10 μ_B (maximum) for different doping elements as mentioned above.

For practical spintronic applications, the Curie temperature (T_C) must be higher than room temperature. The T_C is also calculated using the mean-field approximation for the ferromagnetic cases by using formula^{76, 77}:

$$\frac{3}{2} k_B T_C = - \frac{E_{\uparrow\uparrow} - E_{\uparrow\downarrow}}{N_{TM}} \quad (1)$$

Where $N_{TM} = 2$ is the number of TM impurities in the supercell⁷⁸. By using the formula, the Curie temperature is recorded higher than the room temperature which propose the possibility of transition metal doped plumbene for spintronics application.

4.3 Mechanical Properties

As of late, molecular dynamics simulations under tensile loading, is used to assess plumbene's mechanical characteristics. The mechanical properties of plumbene sheets i.e. ultimate tensile strength and Young's modulus is calculated as 12–17 MPa and 16 GPa respectively which is predominant than bulk lead. These values of Young's modulus and ultimate tensile strength have been estimated under various temperatures and strain velocity formations and are found to be larger than bulk lead^{75,79}.

Henceforth, Plumbene with high mechanical stability may be used as reinforcing agent to improve various nanocomposite having high strength and exceptional material properties⁸⁰⁻⁸⁹.

5. Challenges and conclusion

The absence of process in effortless synthesis techniques has restricted the exploratory developments to help the majority of the theoretical predictions. As of now,

the existing synthesis approaches in fabricating Group IV elemental materials, similar to graphene, have been restricted to substrate reinforce epitaxial growth. Such constraint is anticipated because of the metastable nature of these elemental sheets. Other methods to provide such 2D sheets and cutting them off their growth substrates are however to be investigated. In that capacity, developments in synthesis techniques for generating 2D elemental sheets resembling graphene will be a huge achievement proceeding their enormous possibility for the advancement of another era of electronic, optoelectronic and spintronic applications. Undoubtedly, altogether cases, developing a synthesis method which is cost effective and finding a suitable semiconducting or insulating substrate for IV group 2D materials growth on a large scale stay challenging tasks for technological applications.

Thus, clearly, these 2D materials are guaranteed to a splendid future. However, the indication so far is encouraging. Up until now, plumbene seems to be like the next big thing in two-dimensional materials. Plumbene could be a possible candidate for processes related to high temperature applications and as a topological insulator. In comparison to graphene and silicene, plumbene has invaluable special properties due to its structural configurations too. Indeed, it has prevalent characteristics that can be useful for the functions related to machine traditional lead is utilized so far. Plumbene can too utilized for power generations, preparation of plumbene-reinforced manufacturing, shipbuilding, and in batteries etc., wherein nanocomposites, etc. Plumbene will have anticipated uses wherein conductivity is the major issue.

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