مجلة كلية التربية الاساسية
كلية التربية الاساسية – الجامعة المستنصرية
Journal of the College of Basic Education Vol.29 (NO. 121) 2023, pp. 33-47

Two-dimensional GaP monolayer with tunable electrical and optical properties

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Abstract:

The optical characteristics of two-dimensional (2D) monolayer formations in GaP. According to the predicted binding energies, the GaP monolayers are in constant contact. GaP monolayer was revealed to be semiconducting, with gaps of 2.080 eV. Furthermore, the predicted optical properties indicate that the GaP monolayer will absorb light at wavelengths ranging from infrared to ultraviolet. As a result, GaP monolayer should be appealing for visible-light communication and photocatalytic devices. It is possible to determine that this layer is kinematically stable by studying the form of the phonon, as all frequencies have positive values and there are no negative values for frequency. It is also worth noting that the frequency values exceed 1150 cm^{-1}. Finally, the unexpectedly good properties of GaP monolayer are expected to be used in a variety of combinations in solar cells, field-effect transistors, catalysts, and optical devices.

Keywords:
GaP, the phonon, Optical properties, Electronic properties, two-dimensional (2D), wavelengths.
Note: The research is based on a PhD dissertation.

1. Introduction:

Semiconductors have been at the vanguard of device advances that have resulted in the largest revolution in the last 50 years, and semiconductor research is now concentrated on single crystals. Due to their unique optical

and electrical properties, two-dimensional (2D) materials have rapidly emerged since the discovery of graphene [1]. Because of its extraordinary properties, particularly its great mobility, graphene has emerged as a potential material for optoelectronic applications [2]. Graphene, on the other hand, is unsuitable for optoelectronic applications due to its energy-free band gap [3, 4]. As a result, researchers have been attempting to enlarge the graphene energy gap in order to generate a highly efficient energy gap suitable for optoelectronic applications.

Recently, researchers discovered a number of 2D materials with strong sunlight absorption surfaces, excellent mechanical performance, and huge surface area to volume ratios that might lead to improved optoelectronic applications [5-8]. [9-13] 2-D and 6-D semiconductors (phospholene, antimony, germanene, silicene, and other compounds), methylenes (transition metal nitrides and carbides) [14, 15], metal chalcogenides (MMCs) (GaS, GaSe, InS, and InSe) [16-19] (PDF) [15]. Dichalcogenides (MDCs) (SnS2, SnSe2) [20, 21], Janus monolayers [26, 27], and transition metal dichalcogenides (TMDs) such as MoSe2, MoS2, WSe2, WS2, PtSe2, PtS2 [22-25] are examples of 2D materials. Furthermore, 2D TMDs with properties distinct from ordinary semiconductors are intriguing materials for improving device performance and developing new applications not possible with other monolayers [26-29]. GaP monolayer have attracted a lot of attention as a promising material for improved photovoltaic and electro-electrodevices due to their distinct properties. It's worth noting that GaP monolayers have almost linear bandwidth. A 2 eV gap, which corresponds to the solar spectrum [30,31]. They may also be employed as optical and optical materials because to their high mobility [32-35]. This layer is a semiconductor with a 1.204 eV to 2.080 eV indirect energy gap [37].

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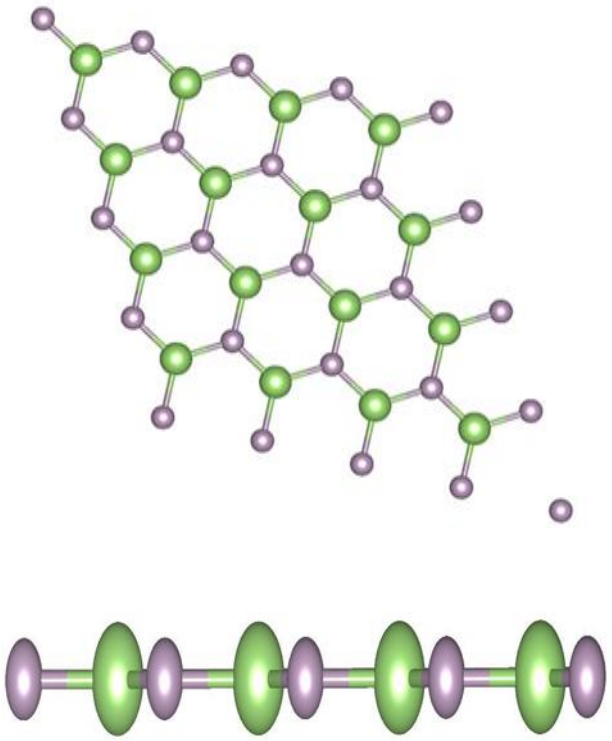


Fig. 1. Top and side views of GaP monolayer [37].

The optical absorption edge can be enlarged in the visible light range [38]. Furthermore, because monolayer structures with different semiconductors can usually prevent photo-induced carrier recombination and change the band gap [39], vdW monolayer structures have the potential to be promising materials. By combining two monolayer materials to generate two-dimensional monolayers, optoelectronic characteristics are improved, and it is commonly utilised in strain sensors, bipolar transistors, and solar cells. Additionally, the electronic structure of monolayers can be altered by varying the materials, layer thicknesses [40], doping [41,42], and layer stacking operations [43-45].

2. Computational details:

The density functional theory (DFT) simulations were performed using the Cambridge Total Energy Package (CASTEP) series [36,46]. Cross-correlations were treated as either monolayer-free or variance-corrected vdW (monogeneous structure) using the Perdew-Burke-Ernzerhof (PBE) function [47-50] or as generalised gradient approximation (GGA) using the DFT-D2 technique [51,52]. Supersmooth pseudopotentials were used to determine the

valence electronic interactions. The Broyden-Fletcher-Goldfarb-Schanno (BFGS) approach was used to smooth all lattice parameters and atomic positions [43]. The plane wave cutoff energy was set at 500 eV, and the Koelling-Harmon function was used for proportional processing.

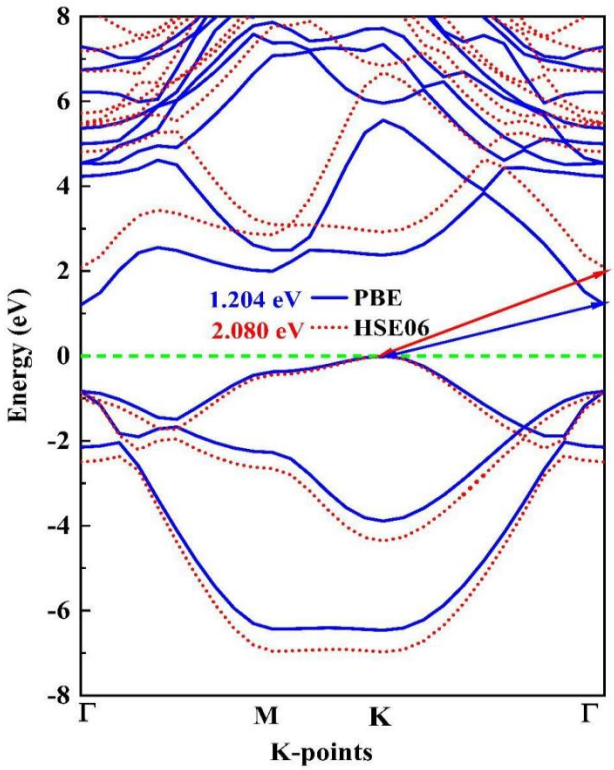


Fig. 2. GaP monolayer electronic band structures. The horizontal red dashed line denotes the Fermi levels.

3. Results and discussion

3.1. Electronic and structural properties:

We started looking for GaP monolayer structure by improving the architectures presented in Fig. 2. GaP has a lattice constant (a) of 3.919 Å and a bond length of (2.262), which is consistent with prior findings [53,54].

The calculated direct band gap of GaP is 2.080 eV, which is less than previously projected theoretical values [55-57], and this value is in the visible light range, hinting optoelectronic applications, however the valence band maximum (VBM) is at the K point and the conduction band minimum (CBM) is at the M-K point.

Fig.3, shows that the highest contribution is in the conduction band representing the positive part, which comes from the 4p orbital of Ga, the 4s

orbital of Ga and a little bit of the 3p orbital of P, while in the valence band representing the negative part, the highest contribution comes from the 3p orbital of P, and a little bit of the 4p orbital of Ga.As for the black color in fig.3, it represents the sum of the contributions, i.e. the total density of states.

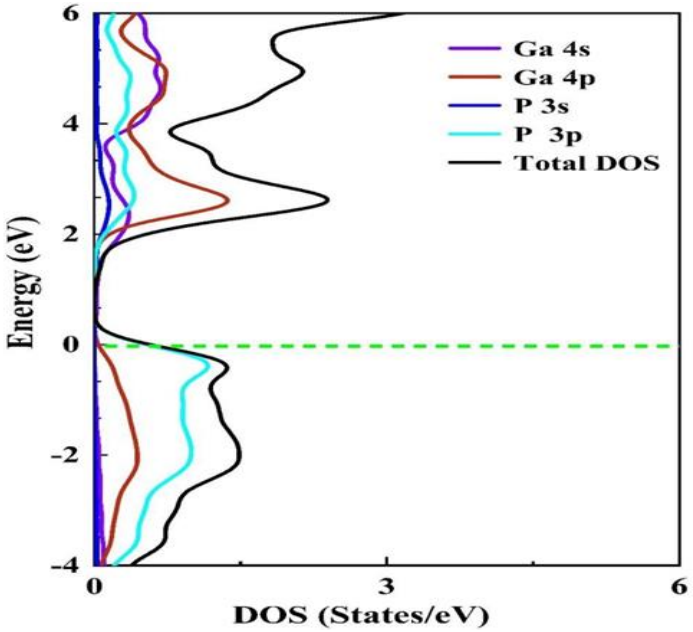


Fig. 3. TDOS of Gap monolayer. The Fermi levels are marked by the vertical dashed line.

3.2 Optical properties:

Understanding the behaviour of materials necessitates knowledge of their optical characteristics. By observing the shape of the phonon, Fig. 4, it can be confirmed that this layer is dynamically stable, as it is noted that all frequencies have positive values and there are no negative values for frequency. It is also noted that the frequency values reach 1150 cm-1. cteristics. This is owing to their importance in understanding how materials behave when they interact with light. Particularly sensitive to light are 2D monolayers.

Figure 5 depicts the greatest peaks of reflectance, absorption, refractive index, and dielectric function for GaP monolayers. The maximum peaks of reflectance and absorption for GaP are 0.102 at 9.26 eV and 9.93*104 at 9.15 eV, respectively; the real image and image of the maximum peak of refractive index are 1.59 at 6.04 eV and 0.675 at 9.07, respectively; and the

real image and image of the maximum peak of dielectric function are 2.46 and 1.52 at 5.95 eV and 8.86 eV, respectively. The real part represents the energy margin, and it is well known that polarizability decreases as photon energy increases. The real dielectric function is obviously negative, causing GaP single crystals to behave like metals.

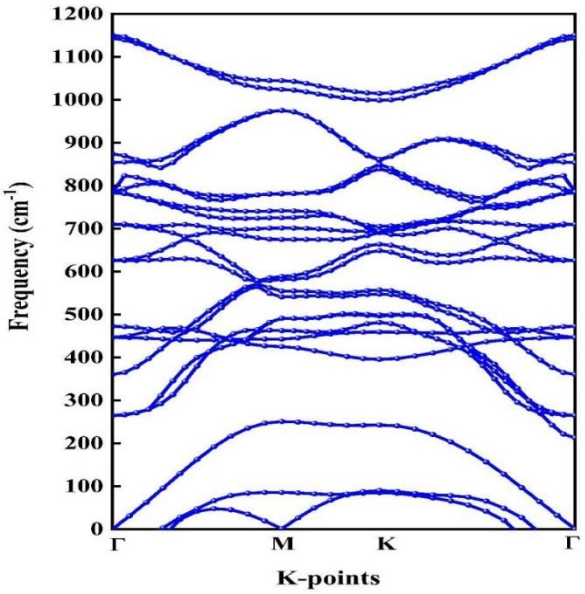
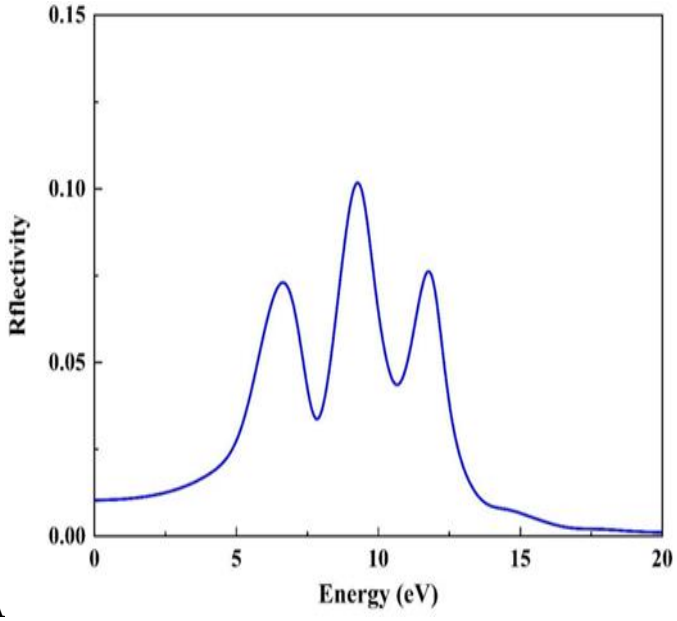
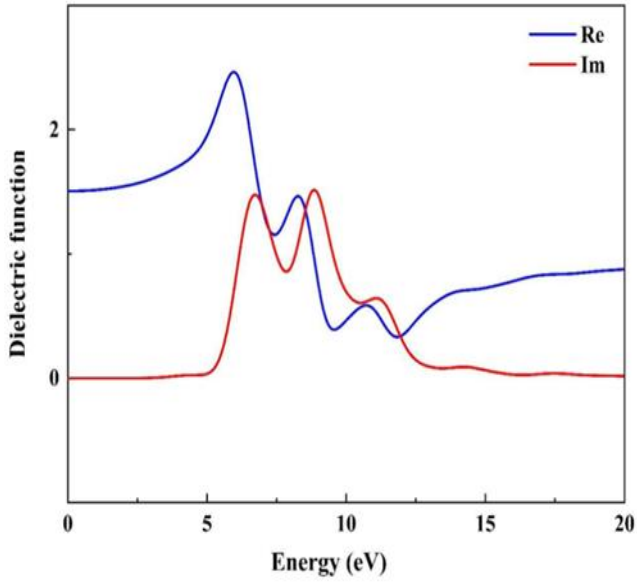


Fig. 4. The phonotical dispersion curve of GaP monolayer.



A


Re
Im
Dielectric function
2
0
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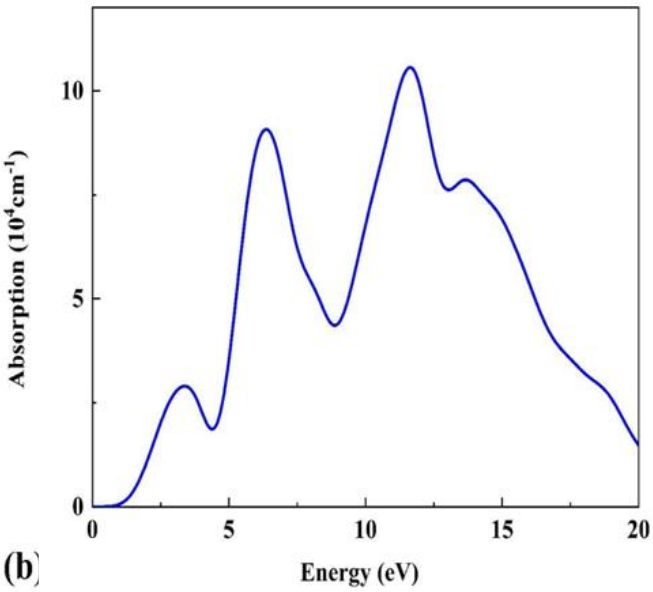
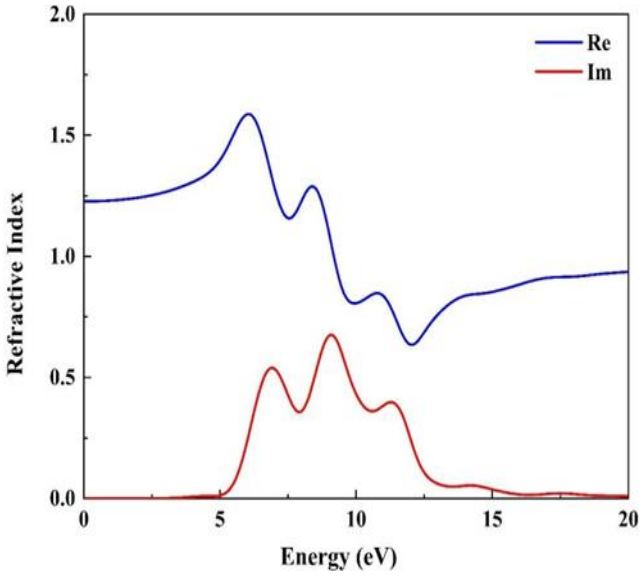
5
10
15
20
Energy (eV)

B


Absorption ($10^4 cm^{-1}$)
10
5
0
0
5
10
15
20
Energy (eV)

C (b)



D

Fig. 5. The optical properties of GaP (A, B, ,C and D) monolayer.

4. Conclusion:

Finally, the structural and optoelectronic properties of GaP monolayer was investigated using dispersion-corrected DFT calculations. The results reveal that the contact between isolated GaP monolayers is simple to build. Monolayers may be readily formed since all linkages are present. Negative energy exist in these different substances. However, GaP monolayers can absorb light at wavelengths ranging from infrared to ultraviolet, and their absorption coefficients are comparable to those of perovskites. As a result, the monomeric structures investigated are likely to be employed in solar cells in these areas. Furthermore, the maximum conductivity and reflectance values in the UV region. The suggested results allow these monomeric structures to be used in electrical and optical applications.

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مجلة كلية التربية الاساسية
كلية التربية الاساسية – الجامعة المستنصرية
Journal of the College of Basic Education Vol.29 (NO. 121) 2023, pp. 33-47

أحادي الطبقة Gap ثنائي الأبعاد ذات الخواص كهربائية وبصرية قابلة للضبط

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المستخلص:
الخصائص البصرية للتكوينات أحادية الطبقة ثنائية الأبعاد (2D) في GaP. وفقًا لطاقات الربط المتوقعة ، تكون الطبقات الأحادية GaP على اتصال دائم. تم الكشف عن أن أحادي الطبقة GaP هو شبه موصل ، مع وجود فجوات تبلغ 2.080 الكترون فولت. علاوة على ذلك ، تشير الخصائص البصرية المتوقعة إلى أن طبقة GaP الأحادية سوف تمتص الضوء بأطوال موجية تتراوح من الأشعة تحت الحمراء إلى الأشعة فوق البنفسجية. نتيجة لذلك ، يجب أن يكون GaP أحادي الطبقة جذابًا لاتصالات الضوء المرئي وأجهزة التحفيز الضوئي. من الممكن تحديد أن هذه الطبقة مستقرة حركيًا من خلال دراسة شكل الفونون ، حيث أن جميع الترددات لها قيم موجبة ولا توجد قيم سالبة للتردد. وتجدر الإشارة أيضًا إلى أن قيم التردد تتجاوز 1150 سم $^{-1}$. أخيرًا ، من المتوقع استخدام الخصائص الجيدة بشكل غير متوقع لـ طبقة GaP الأحادية في مجموعة متنوعة من التوليفات في الخلايا الشمسية ، والترانزستورات ذات التأثير الميداني ، والمحفزات ، والأجهزة البصرية.

الكلمات المفتاحية: GaP ، الفونون ، الخصائص البصرية ، الخصائص الإلكترونية ، ثنائي الأبعاد (2D) ، الأطوال الموجية.

ملاحظة : هل البحث مستل من رسالة ماجستير او اطروحة دكتوراه ؟ نعم مستل من اطروحة دكتوراه