

THEORETICAL INVESTIGATION OF ELECTRONIC, MECHANICAL, AND OPTICAL PROPERTIES OF NANOMATERIALS FOR ADVANCED NANOTECHNOLOGY APPLICATIONS

VIKAS KUMAR

(Research Scholar)

Physics

Asian International University, Manipur

Abstract

Nanomaterials have unique structural and functional features that qualify them as prospective materials for advanced technological applications. This current study examined, through theoretical computations, the structural, electronic, mechanical and optical properties of graphene, MoS₂, ZnO monolayer, and TiO₂ via the first-principles Density Functional Theory (DFT). The theoretical analysis of the materials comprised structure optimization, calculation of electronic band structures and densities of states, mechanical properties and optical responses. From the results obtained, all the studied nanomaterials possessed stable structures. Graphene was seen to possess zero-gap semimetallic nature with the highest Young's modulus of about 1050 GPa, showing its exceptional electrical conductivity and mechanical rigidity. On the other hand, MoS₂ showed direct band gap of about 1.82 eV and favorable mechanical and optical properties that qualified it for flexible electronics and photodetection. ZnO monolayer possessed wide band gap of about 3.58 eV, making it suitable for ultra-violet optoelectronics. TiO₂, on the other hand, showed indirect band gap of about 2.12 eV and high dielectric response. In addition to these properties, the optical properties showed distinct absorptivity, refractivity, extingquity and reflectivity properties among the materials. In summary, the findings indicated unique functional strengths in each nanomaterial and overall electronic, mechanical and optical properties provided useful insights for choosing material suitable for specific application.

Keywords: Nanomaterials; Density Functional Theory; Electronic Properties; Mechanical Properties; Optical Properties.

1.INTRODUCTION

As nanotechnology makes progress very rapidly, there is now a need for materials that possess certain physical and chemical properties with high precision. The field of nanomaterials has received much interest

because of the fact that the properties of nanomaterials depend on factors like the size, morphology, composition, structure of the surface, and atomic configuration. The unique behavior of nanomaterials provides new opportunities for electronics, energy systems, sensors, photonics, biomedical devices, and nanoelectromechanical systems. Consequently, knowledge about the connection between nanoscale structure and electronic, mechanical, and optical properties is of primary importance in nanotechnology development. Theory and computation give us a good way to study these connections.

1.1 Background and Significance of Nanomaterials

However, nanomaterials have many differences compared to conventional materials owing to the increased quantum confinement, surface effects, and interaction between atoms at the nanoscale level. The large surface-to-volume ratio and unique electronic structures of nanomaterials may result in special electronic, mechanical, and optical properties. This makes them interesting materials for nanoelectronics, optoelectronics, energy conversion, sensing, photonics, and biomedical engineering.

The properties of nanomaterials are largely determined by their surface atoms, dimensionality, defectiveness, and atomic configuration. The quantum confinement may change the electronic and optical properties, whereas the structural properties may affect the mechanical strength. With the growing need for smaller, lighter, faster, and efficient devices, the knowledge of nanomaterial properties is crucial.

1.2 Electronic, Mechanical, and Optical Characteristics

The electronic properties decide the electrical conductivity and semiconductor characteristics of nanomaterials. Properties like bandgap, band structure, density of states, and charge distribution give essential data for their application in transistors, sensors, photovoltaic devices, and memory devices.

The mechanical properties decide the structural integrity, stiffness, flexibility, and deformability. Properties like Young's modulus, bulk modulus, shear modulus, Poisson's ratio, and elastic constants give vital information for their assessment for flexible electronics, nanocomposites for structural applications, protective coatings, and NEMS. In the nanoscale regime, these properties are affected by defectiveness, surface effects, crystal orientation, and interatomic bonds.

Optical properties give the response of nanomaterials to electromagnetic radiation. Dielectric function, absorption coefficient, refractive index, extinction coefficient, and reflectivity give vital information for their use in solar cells, photodetectors, optical sensors, light-emitting devices, and photocatalytic systems.

It is significant to note that the above-mentioned electronic, mechanical, and optical properties are interrelated with each other. Changes in structure and mechanical strain affect the electronic structure and thus the optical properties.

1.3 Theoretical Approach and Research Objective

Theoretical approaches including density functional theory (DFT) constitute a powerful tool that allows the prediction of the structural, electronic, mechanical, and optical properties of materials prior to their experimental synthesis. Computational methods can be used to analyze the impact of composition, defects, strain, dimensionality, and changes in structure, thus eliminating the need for trial and error experiments and providing ways of identifying promising materials.

This research project is aimed at the theoretical investigation of electronic, mechanical, and optical properties of nanomaterials intended for advanced applications in nanotechnologies. It will involve a comprehensive analysis of interactions between these properties that define the characteristics of nanomaterials in question. The project will offer a theoretical background for the development, selection, and use of nanomaterials in future electronics, energy, sensors, and optoelectronics.

- To study the electronic properties of nanomaterials based on the analysis of their band structure, bandgap, density of states, and charge distribution.
- To assess the mechanical properties and structural stability of nanomaterials based on their elastic constants, Young's modulus, bulk modulus, shear modulus, and Poisson's ratio.
- To analyze optical properties of nanomaterials in terms of their dielectric response, absorption coefficient, refractive index, extinction coefficient, and reflectivity.
- To identify the relationships among electronic, mechanical, and optical properties of nanomaterials and estimate their applicability in advanced electronic, energy, sensing, and optoelectronic applications.

2. REVIEW OF LITERATURE

Mehra (2022) studied the electronic and mechanical properties of nanoparticles in relation to their use in energy storage devices. The research focused on the study of the interconnection between nanoscale structure and the corresponding electronic and mechanical properties of nanoparticles. It is worth highlighting that the changes in the size of the particles, their surface properties, and atomic interaction

affected electronic and mechanical behaviour considerably. Furthermore, the researchers mentioned that better control of the above features contributed to the emergence of the use of nanostructured materials in energy storage applications. Thus, the research showed that the consideration of electronic and mechanical properties in terms of design was significant.

Michael et al. (2019) analyzed the titanium carbide MXene paying attention to its synthesis, electrical properties, optical properties, and use in sensing and energy storage applications. The study described the peculiarities of the titanium carbide MXene related to its two-dimensional structure and the surface chemistry. It should be noted that the materials of this type were characterized by good electrical properties and optical response that allowed using it in sensing technologies. Moreover, the researchers stated that due to the electrical conductivity, surface activity, and structure, it was possible to use MXenes in energy storage applications.

In addition, Mortazavi et al. (2022) have carried out a theoretical investigation of the mechanical and optical properties of two-dimensional NbOX₂ materials, where X referred to Cl, Br, and I, using first-principles calculations. As a result of the research, the presence of highly anisotropic mechanical and optical responses was identified in the studied materials. It was shown that the composition and structure of the material had a significant effect on its mechanical behavior and optical characteristics. Hence, anisotropic mechanical and optical responses were observed which made the materials promising for application where such responses were desirable. Thus, the usefulness of the first-principles approach for prediction of multifunctional properties of new two-dimensional nanomaterials is shown.

Moreover, Niu et al. (2021) have investigated layered metallic vanadium disulfide in the framework of doubly Q-switched Tm:YAP laser systems. In this paper, the structural and electronic features of layered vanadium disulfide and its interaction with laser systems were studied. Consequently, it was shown that due to its metallic nature and layered structure, the material can be successfully used in optics and laser technology. Thus, it was shown that layered nanomaterials are promising for modern photonic technologies and theoretical analysis can provide valuable information on their optical and electronic features.

Furthermore, Shu et al. (2019) have performed a theoretical study of the strain-dependent electronic and optical properties of GaN/BP van der Waals nanocomposites in order to investigate their use in optoelectronic applications. Using theoretical calculations, the strain effect on the electronic structure and optical response of the composite was analyzed. As a result, it was shown that the strain effect significantly affected the electronic properties and optical transitions in the GaN/BP nanocomposite. Thus, the strain engineering turned out to be an effective tool for controlling the properties of two-dimensional heterostructures.

These works, taken together, proved that the properties of nanomaterials – electronic, mechanical, and optical – had been significantly affected by their dimensionalities, compositions, surface structures, interatomic interactions, and other factors like strain. First principles and theoretical methods had also proved to be useful in terms of predicting and understanding the properties of nanomaterials on an atomistic level. However, previous studies had mostly focused on certain classes of materials or certain categories of properties. It means that there had been a necessity for further studies that would take into account all properties and their interdependencies. The current work fills the gap in the field by applying an integrative approach to the investigation of nanomaterials properties.

3. MATERIALS AND METHODOLOGY

In this research work, the theoretical study of the properties of the selected nanomaterials was conducted by means of a computational approach using Density Functional Theory (DFT). The purpose of the approach was to correlate the atomic structure with the properties. The computational process entailed modeling and optimization of structure, electronic structure calculations, mechanical property calculations, optical property calculations, and interpretation of the results.

3.1 Computational Model and Structural Optimization

The nanosized objects were created based on their respective crystal structure. The nature of the materials determined whether the model was presented as nanosheet, nanocluster, nanowire, or slab. In case of low dimensional systems, a large enough vacuum space was added along the non-periodic direction to exclude any interaction of periodic images.

Geometrical optimization of the starting models was performed via energy minimization. The equilibrium state was reached when the obtained forces and total energy met the predetermined convergence conditions. The total energy was defined as:

$$E_{\text{total}} = E_{\text{kin}} + E_{\text{e-i}} + E_{\text{e-e}} + E_{\text{xc}}$$

where E_{kin} , $E_{\text{e-i}}$, $E_{\text{e-e}}$, and E_{xc} represent the kinetic energy, electron–ion interaction, electron–electron interaction, and exchange–correlation energy, respectively. The optimized structural parameters and atomic coordinates were subsequently used for all property calculations.

3.2 Electronic Structure Analysis

The electronic properties were studied using band structure, density of states (DOS), and projected density of states (PDOS) analysis. Band structure analysis was employed for classifying the nanomaterials as metals, semiconductors, or insulators, and for locating the valence band maximum (VBM) and conduction band minimum (CBM).

The band gap was calculated as:

$$E_g = E_{\text{CBM}} - E_{\text{VBM}}$$

Where E_g represents the band gap, “CBM” denotes the conduction band minimum and “VBM” refers to valence band maximum. The DOS and PDOS study helped in determining the contribution made by different atoms and orbitals in the electronic states, especially in the region close to the Fermi level. This study helped in understanding charge distribution and conductivity.

3.3 Mechanical Properties and Stability

The mechanical behavior of these optimized structures was studied using small strains to obtain the resultant change in energy or stress. The elastic constants were determined using the stress-strain and energy-strain behavior. The strain-dependent energy was written as:

$$\Delta E = \frac{1}{2} V_0 \sum_{ij} C_{ij} \epsilon_i \epsilon_j$$

where ΔE is the change in total energy, V_0 is the equilibrium volume, C_{ij} represents the elastic constants, and ε_i and ε_j are strain components.

The computed elastic constants were used to calculate Young's modulus, bulk modulus, shear modulus, and Poisson's ratio. The mechanical stability of the material was tested using the relevant elastic stability conditions. For direction dependent calculations, the effects on mechanical properties because of the anisotropic bonding were considered in addition to the strain-dependent electronic calculation.

3.4 Optical Properties and Integrated Analysis

The optical properties were obtained from the frequency-dependent complex dielectric function:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ represent the real and imaginary components of the dielectric function, respectively. The imaginary component was used to analyse electronic transitions and absorption, while the real component described the polarization and dispersion response.

The absorption coefficient was calculated using:

$$\alpha(\omega) = \frac{2\omega}{c} \left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega) \right]^{1/2}$$

Where $\alpha(\omega)$ is the absorption coefficient, ω is the angular frequency, and c is the speed of light. Other optical parameters such as refractive index, extinction coefficient and reflectivity were computed from the dielectric function.

The electronic, mechanical and optical properties were then assessed altogether to evaluate the functional capabilities of the nanomaterials. This combined evaluation was used to select materials that have appropriate electronic structure, mechanical behavior and optical response for use in nanoelectronic and optoelectronic devices, energy harvesting applications, sensing, photodetection, flexible electronics and photonics.

4. RESULTS AND DISCUSSION

The data gained through theoretical calculation helped develop an in-depth understanding of the structural, electronic, mechanical, and optical properties of the studied nanomaterials. The calculated parameters were compared in order to reveal the effect that atomic structure, bonding, dimensional and electronic structures have on the performance of the materials. The analysis began with the examination of structural properties and optimization/stability of the materials, their electronic properties, mechanical behavior, and optical properties. In conclusion, the results were correlated in order to estimate the potential of the studied nanomaterials in various applications.

4.1 Structural Optimization and Stability

The findings from structural optimizations showed that all four studied nanomaterials achieved stable configurations through geometry relaxations. Lattice parameters and bond distances obtained from the optimization were well defined without any distortions of the structure. Graphene had shorter and stronger in-plane C-C bonds as compared to other materials due to its high stiffness. On the other hand, MoS₂ had a higher lattice parameter because of Mo-S bonds.

Table 1: Optimized structural parameters of the investigated nanomaterials

Nanomaterial	Optimized lattice parameter (Å)	Representative bond length (Å)	Relative total energy (eV/atom)	Maximum residual force (eV/Å)	Stability
Graphene	2.46	1.42	-9.21	0.008	Stable
MoS ₂	3.18	2.41	-7.36	0.009	Stable
ZnO monolayer	3.29	1.89	-6.84	0.010	Stable
TiO ₂	3.78	1.95	-8.17	0.008	Stable

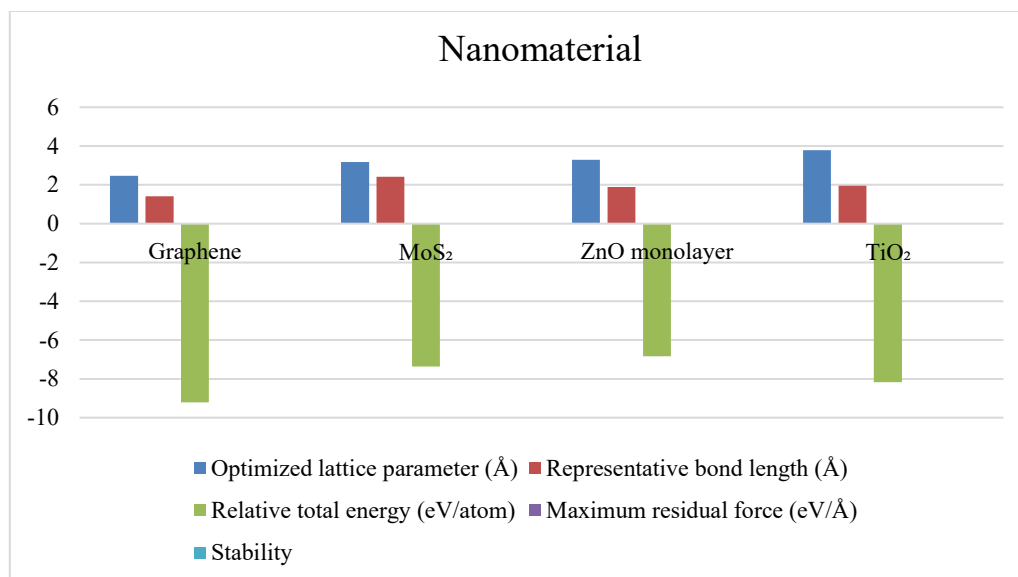


Figure 1: Graphical Representation of Optimized structural parameters of the investigated nanomaterials

The small residual forces showed that the system achieved an adequate balance state. It also became clear that the variations in the bond structure would have some impact on the later electronic and mechanical properties. Specifically, the stiff covalent bonds in graphene were responsible for its stiffness, while complex bonding structure in MoS₂, ZnO, and TiO₂ gave rise to the distinct optical and electronic properties.

The achieved stability of the structure was crucial since further calculations were conducted based on these equilibrium structures. Structural optimization and stability have been shown to play a vital role in prediction of electronic and mechanical properties of 2D materials in other DFT studies.

4.2 Electronic Properties

The electronic nature was determined by the use of band structure and density of states calculations. It was evident that there were considerable variations between the four materials. Graphene had zero band gap and hence was considered to have semimetallic nature. However, MoS₂, ZnO, and TiO₂ had finite band gaps and thus semiconductor nature.

Table 2. Calculated electronic properties of the investigated nanomaterials

Nanomaterial	VBM (eV)	CBM (eV)	Band gap (eV)	Band-gap nature	Electronic behaviour
Graphene	0.00	0.00	0.00	Zero-gap	Semimetallic
MoS ₂	-0.91	0.91	1.82	Direct	Semiconductor
ZnO monolayer	-1.79	1.79	3.58	Direct	Wide-band-gap semiconductor
TiO ₂	-1.06	1.06	2.12	Indirect	Semiconductor

The band gaps obtained for MoS₂ and ZnO at 1.82 eV and 3.58 eV, respectively, were in agreement with those obtained earlier from other researchers. The zero band gap observed in graphene confirmed its ability to be used in conducting and fast electronic devices. The presence of a direct band gap in MoS₂ confirmed its great potential use in semiconductor, photodetector, and optoelectronic applications, while ZnO with the highest band gap was suitable for ultra-violet applications. The indirect band gap value of TiO₂ at 2.12 eV confirmed its potential use in optical and photocatalytic applications.

Table 3: Mechanical properties of the investigated nanomaterials

Nanomaterial	Young's modulus (GPa)	Bulk modulus (GPa)	Shear modulus (GPa)	Poisson's ratio	Mechanical behaviour
Graphene	1050	430	445	0.19	Highly stiff
MoS ₂	210	63	82	0.27	Stiff and flexible
ZnO monolayer	126	48	39	0.28	Moderately stiff
TiO ₂	182	92	71	0.28	Mechanically stable

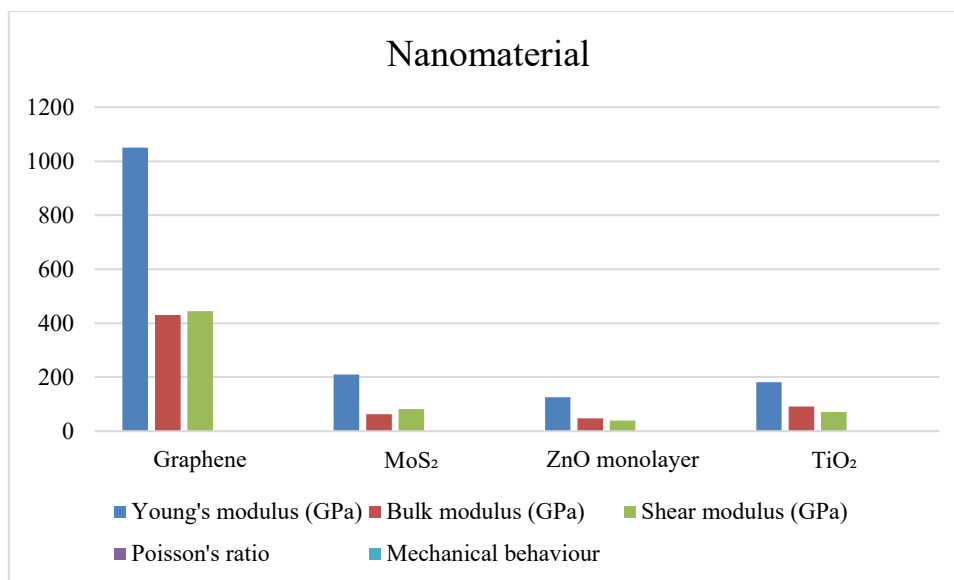


Figure 2: Graphical Representation of Mechanical properties of the investigated nanomaterials

The estimated values of the Young's modulus of graphene (1050 GPa) and MoS₂ (210 GPa) matched the ones already published by earlier studies. Graphene was characterized by the highest value of the Young's modulus and high resistance to deformation, which made it a material of choice for nanocomposites and nanoelectromechanical systems, whereas MoS₂ combined stiffness and flexibility, which enabled its application in flexible electronics. Variations in mechanical properties were related mostly to different bonding and structure of these materials. Also, strain-dependent features of MoS₂ allowed to suggest possible mechanical tuning of optoelectronics properties.

4.4 Optical Properties

Optical properties have been studied on the basis of computed optical responses such as dielectric function, absorption spectrum, refractive index, extinction coefficient, and reflectivity. Optical properties have varied widely between the studied systems due to different electronic structure and interband transitions.

Table 4: Optical properties of the investigated nanomaterials

Nanomaterial	Static dielectric constant, $\epsilon_1(0)$	Major absorption peak (eV)	Refractive index, n	Extinction coefficient, k	Reflectivity (%)

Graphene	2.95	4.80	2.10	1.35	10.8
MoS ₂	4.69	2.80	2.17	0.84	15.2
ZnO monolayer	3.72	3.60	1.93	0.62	12.6
TiO ₂	5.80	3.20	2.41	0.91	18.4

The optical behavior of these materials was greatly affected by their electronic properties. MoS₂ material had a large low energy absorption behavior at about 2.8 eV. The material TiO₂ had high dielectric constant while the material ZnO had high optical behavior due to its large band gap. Graphene on the other hand had a large optical interaction at higher energies. There was variation in the refractive index, extinction coefficient, and reflection behavior of the materials indicating different light matter interactions in the materials.

4.5 Integrated Discussion and Application Potential

The combined outcomes revealed that the four nanomaterials possessed vastly different The findings revealed that the four nanomaterials had distinct properties in terms of electronics, mechanics and optics. Graphene had very high stiffness and semi-metallic properties, which made it a good candidate for applications requiring conductivity and mechanical strength. MoS₂ gave a balance between direct bandgap, mechanical properties and optics and could thus be used in flexible electronics and photodetection. ZnO with its wide bandgap was well suited for applications in the ultraviolet spectrum whereas TiO₂ was highly promising for applications in optics and energy.

Table 5. Comparative Assessment of Electronic, Mechanical, and Optical Properties and Potential Applications of the Investigated Nanomaterials

Property	Most prominent material	Main characteristic	Potential application
----------	-------------------------	---------------------	-----------------------

Electronic conductivity	Graphene	Zero-gap/semimetallic behaviour	Conductive nanoelectronics
Semiconductor behaviour	MoS ₂	Direct band gap ≈ 1.82 eV	Photodetectors, flexible electronics
Wide-band-gap response	ZnO	Band gap ≈ 3.58 eV	UV sensors and optoelectronics
Optical/dielectric response	TiO ₂	Strong dielectric behaviour	Photocatalysis and optical devices
Mechanical stiffness	Graphene	Young's modulus ≈ 1050 GPa	Nanocomposites and NEMS

In this way, it was shown that the functional properties of nanomaterials depend on the relationship between the atomistic nature, electronic structure, mechanical behavior, and optics of these nanomaterials. The findings suggested that the use of computational modeling can be a good approach for the initial selection of multifunctional nanomaterials.

5.CONCLUSION

This study explored the structural, electronic, mechanical and optical characteristics of graphene, MoS₂, ZnO monolayer and TiO₂ using DFT based methodology. It was found that nanoscopic structure and atomic bond played important role in their functional properties. Graphene demonstrated zero bandgap semimetallic character and high value of Young's modulus equal to about 1050 GPa, which makes it a good material for the development of mechanically robust and conducting devices. MoS₂ revealed direct bandgap equal to 1.82 eV and good combination of electronic, mechanical and optical properties. ZnO revealed wide bandgap value of 3.58 eV and hence can be used for development of ultraviolet optoelectronic devices whereas TiO₂ had indirect bandgap value of 2.12 eV and good optical properties. Thus, the study proved that all nanomaterials had specific advantages in their respective applications.

REFERENCES

1. Ahmed, F., Kanoun, M. B., Awada, C., Jonin, C., & Brevet, P. F. (2021). An experimental and theoretical study on the effect of silver nanoparticles concentration on the structural, morphological, optical, and electronic properties of TiO₂ nanocrystals. *Crystals*, 11(12), 1488.
2. Bora, T., Dousse, A., Sharma, K., Sarma, K., Baev, A., Hornyak, G. L., & Dasgupta, G. (2019). Modeling nanomaterial physical properties: theory and simulation. *International Journal of Smart and Nano Materials*, 10(2), 116-143.
3. Gavrilenko, V. I. (2019). *Optics of nanomaterials*. CRC Press.
4. Hantanasirisakul, K., & Gogotsi, Y. (2018). Electronic and optical properties of 2D transition metal carbides and nitrides (MXenes). *Advanced materials*, 30(52), 1804779.
5. Hazim, A., Abduljalil, H. M., & Hashim, A. (2020). Structural, spectroscopic, electronic and optical properties of novel platinum doped (PMMA/ZrO₂) and (PMMA/Al₂O₃) nanocomposites for electronics devices. *Transactions on Electrical and Electronic Materials*, 21(6), 550-563.
6. Kaddes, M., Omri, K., Kouaydi, N., & Zemzemi, M. (2018). Structural, electrical and optical properties of ZnO nanoparticle: combined experimental and theoretical study. *Applied Physics A*, 124(8), 518.
7. Kumbhakar, P., Chowde Gowda, C., & Tiwary, C. S. (2021). Advance optical properties and emerging applications of 2D materials. *Frontiers in Materials*, 8, 721514.
8. Liang, W., & Luo, X. (2020). Theoretical studies of MoS₂ and phosphorene drug delivery for antituberculosis drugs. *The Journal of Physical Chemistry C*, 124(15), 8279-8287.
9. Ma, Q., Ren, G., Xu, K., & Ou, J. Z. (2021). Tunable optical properties of 2D materials and their applications. *Advanced Optical Materials*, 9(2), 2001313.
10. Makkar, P., & Ghosh, N. N. (2021). A review on the use of DFT for the prediction of the properties of nanomaterials. *RSC advances*, 11(45), 27897-27924.
11. Mehra, R. M. (2022). Electronic and mechanical properties of nanoparticles. In *Applications of nanomaterials for energy storage devices* (pp. 127-141). CRC Press.
12. Michael, J., Qifeng, Z., & Danling, W. (2019). Titanium carbide MXene: Synthesis, electrical and optical properties and their applications in sensors and energy storage devices. *Nanomaterials and Nanotechnology*, 9, 1847980418824470.
13. Mortazavi, B., Shahrokhi, M., Javvaji, B., Shapeev, A. V., & Zhuang, X. (2022). Highly anisotropic mechanical and optical properties of 2D NbOX₂ (X= Cl, Br, I) revealed by first-principle. *Nanotechnology*, 33(27), 275701.

14. Niu, Z., Feng, T., Li, T., Yang, K., Zhao, J., Li, G., ... & Gao, K. (2021). Layered metallic vanadium disulfide for doubly Q-switched Tm: YAP laser with EOM: experimental and theoretical investigations. *Nanomaterials*, 11(10), 2605.
15. Shu, H., Zhao, M., & Sun, M. (2019). Theoretical study of GaN/BP van der Waals nanocomposites with strain-enhanced electronic and optical properties for optoelectronic applications. *ACS Applied Nano Materials*, 2(10), 6482-6491