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Quasi-particle band structure and optical properties of Perylene Crystal for Solar Cell Application: A G_0W_0 Calculations

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Abstract: *The increased demand for clean energy due to future fear of scarcity and alarming pollution threats from fossil fuels, has propelled stringent drive on the search for alternative energy source including photovoltaic technology. This technology relies on renewable source and is green, eco-friendly and easily avoidable. In view of the role of photovoltaic technology on organic compound for electronic transition, this study is designed to implement theoretical calculations of structural, electronic and optical properties of the perylene crystal using highly accurate first-principles approach for a many-body perturbation theory (MBPT). The calculated lattice parameters of perylene with GGA-PBE are reasonably in good agreement with experimental measurement. Many-body perturbation theory (MBPT) based on the G_0W_0 approximation was used for the calculation of band structure. The bandgap value of 2.4 eV, obtained was consistent with the expected range from experiment (i.e, 2.33-2.46 eV). The optical properties including absorption coefficient, reflectivity, refractive index and energy loss function are derived from the calculated complex dielectric function to understand the optical behavior of perylene. Optical properties calculations show that the results obtained within G_0W_0 approximation are also close to experimental results. With the evaluated optical gap of 2.4 eV and the expected strong absorption of perylene crystal in the visible light, the investigated material is most likely suitable for solar cell application.*

Keywords: *Solar cell, Perylene, DFT, G_0W_0, Yambo, bandwidth, optical absorptiom*

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1.0 Introduction

Year by year, the demand for clean energy to minimize the emission of greenhouse gases that have threatened the catastrophic changes in global climate is on the increase (Hao & Shao, 2021). Many extensive efforts were done and (and is ongoing) to overcome the problem. Photovolaic technology is one of the most reliable and attractive approaches. The technology harvests the solar energy by converting solar radiation to electricity directly (Cavallaro, Zavadskas, Streimikiene, & Mardani, 2019; Lawal, Shaari, *et al*., 2021). By providing approximately 10^4 times larger energy than our present needs, the solar energy is expected to be the best solution to the existing problems in the energy or power sector (Boza & Evgeniou, 2021). Global industrial sectors have led to the exploitation of photovoltaic technologies that rely upon inorganic materials such as silicon (Ebhota & Jen, 2020). The inorganic materials have been

proved to perform well in photovoltaic device (Noel *et al*., 2014). However, several disadvantages in terms of high cost and limited resources have sparked the interest among researchers to explore and investigate the replacement for the material (Kiran, Preethi, & Kumar, 2022; Noel *et al.*, 2014). Therefore, current research attention is focussed on the application of organic materials as solar cells in photovoltaic applications. By offering some advantages such as; low cost, light, flexible, thin, available in abundance, sustainable, and others. Organic photovoltaic (OPV) application has received extraordinary scientific and industrial attention recently. One of the organic materials that have attracted the attention of both the academic and the industrial community for photovoltaic application is perylene crystal, due to its nature and physical properties such as high stability, high solubility, high efficiency and other factors that enhance its suitable as an electron acceptor material. (Lai *et al.*, 2015). Its polycyclic hydrocarbon construction with the conjunction of single and double bonds points out the presence of high charge population in it, which is accurately attributed to the presence of weak π−π interaction within the perylene crystal structure (Kumagai *et al*., 2022). The history of perylene crystal structure was pioneered by Donaldson, Robertson and White (1953) . However, the accuracy of the two bonds connecting the two naphthalene nuclei was not well resolved. Hence several years later, the exact values of the two connector bonds were finally found to be longer (1.50 Å) from the actual value of the expected molecular symmetry (Camerman & Trotter, 1964). The molecular crystal of perylene has earnestly been studied either through α or β crystalline phase and has shown its electronic potential as an active material for OPV as it can be seen through its outstanding properties in several studies (Lane *et al*., 2000; Sugiyasu, Fujita, & Shinkai, 2004). Yiding Lai *et al*. (2015), concluded the shape of the crystals must be taken into account, as different shapes of perylene crystals can realistically affect the findings as shown in some perylene UV−vis absorption spectra. Rapid inventions and findings on perylene crystal have existed starting in 2007, with the discovery of Di-indeno perylene (DIP) by Michael A. Heinrich *et al*. (2007). DIP crystal structure compromised with a different arrangement of molecules leads to different behavior of photons and electrons, and consequently, different outcomes were observed. The relation of the building block of molecules up to organic molecular crystal is predicted to influence the system performance. Hence, it is important to evaluate the relations of molecule-crystal. According to Liao *et al.* (2014), most of organic molecular crystals are structure-dependent, although the relationship may be not be easily explored or computed in the gas or condensed phases. Hence, most of the relation still remains elusive. This suggests theoretical approach is preferable in order to evaluate the respective study. Therefore, in order to attain its respective properties, a comprehensive investigation on the structure, electronic and optical properties are needed. In this regard, the use of first-principles approach in performing virtual experiment may lead to a cheaper experiment and shorter developmental cycle. First-principles calculation based on density functional theory (DFT) are intensely used by the theoretical researchers to solve the complex problems. However, electronic band gap and optical gap are usually underestimated within such method. Hence, to overcome this inconsistency between DFT calculation and experimental results, one-particle Green's function based on many-body perturbation theory (MBPT) within non-self-consistent GW approach (one-shot G_0W_0 approximation) is one of the most reliable and cheapest method for computing quasiparticle (QP) band structure/bandgap closer to the experimental value. In this work, structural, electronic and optical properties of Perylene are performed within the framework of DFT in combination of G_0W_0 approximation as implemented in Quantum Espresso and YAMBO codes.

2.0 Computational details

In this work, all calculations were performed with Quantum Espresso (Giannozzi *et al*., 2009) and YAMBO (Marini, Hogan, Grüning, & Varsano, 2009) simulation codes. Quantum Espresso (QE) is a software for materials modelling and electronic structure calculations based on pseudopotential DFT formalism (Giannozzi *et al*., 2017). Also, QE interface with YAMBO was used for excided state calculation using DFT results as its input. Yambo simulation package is a code designed for calculating quasi-particle (QP) energies and optical properties within many-body perturbation theory (MBPT) (Lawal, Shaari, Ahmed, & Jarkoni, 2017; Sangalli *et al*., 2019). Quasi-particle energies were calculated within the one-shot G_0W_0 approximation. The optical absorption spectra were computed with YAMBO code. Yambo code is chosen in this study because of known accuracy for band structure and optical properties calculations. Accuracy in band gaps with this approach with experimental measurements is due to many-body perturbation theory (MBPT) by the QP concept. Optical properties calculations using Yambo code for a number of systems in several studies show high accuracy approaching experimental values. Electronic structure and optical properties of perylene crystal calculations were performed based on Pseudopotential plane-wave method. Perdew-Burke-Ernzerh of generalized gradient approximation (PBE-GGA) exchange-correlation potential is used for lattice dynamics of perylene crystal (Perdew, Burke, & Ernzerhof, 1996) Norm-conserving pseudopotential were used in modelling interaction between ionic core potential and electron of H and N atoms. The Brillouin zone integration was performed using Monkhorst-Pack grid of k-points grids for structural and band structure calculations. 70 Ry cut-offs energy of the plane-wave basis set was used to expand the wave functions and 450 Ry for charge density. Quasiparticle band structure and optical properties of perylenecrystal were calculated by G_0W_0 approximation for the self-energy operator. Specifically, frequency dependence of the dielectric matrix was treated by single one shot G_0W_0 approximation via Godby-Needs plasmon pole model. In the one-shot calculations, Converged results attained by kinetic energy cut-offs of 24 Ry for screening dielectric function with 2000 bands.

3.0 Results and discussions

3.1 Structural properties of perylene

Geometrical relaxation is the first step in any first-principles calculation to avoid a certain error for accurate predictions of other quantities such as electronic band gap and optical spectra. Computationally, geometry optimization is a process whereby atomic coordinates and cell parameters are adjusted, so that the total energy of the structure is minimized to the most stable state and gradient approaching zero. Complete optimization processes will provide a stable geometry. In the perylene study, a crystal of Di-indenoperylene (DIP) has been chosen to represent the crystal of perylene. Figure 1 shows the schematic diagram of perylene crystal in the primitive-centered monoclinic lattice with space group of P21/c. Perylene crystal contained 64 carbon atoms and 32 hydrogen atoms. The obtained lattice parameters of perylene crystal with GGA-PBE were found to be a = 7.1709Å, b = 8.5496Å, c = 16.7981Å with an angle of β = 92.416°. These values are found to be agreed well with the previous studies (Heinrich *et al.*, 2007).

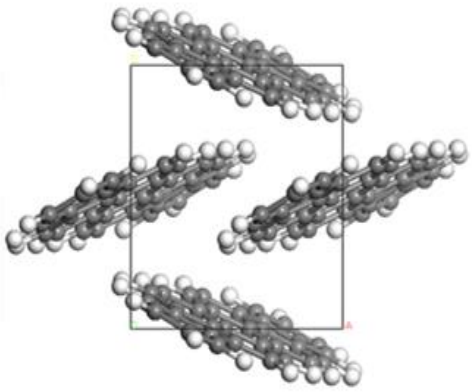

Fig. 1: Graphical view of DIP single crystal of perylene where grey and white balls represent carbon and hydrogen atoms

3.1 Electronic properties of perylene

Electronic properties play important role in describing the performance of OPV materials. Electronic properties are mostly determined by the energy gap between conduction and valence band. The energy gap will indicate the tendency for an electron to move from the highest occupied molecular orbital (HOMO) to the lowest occupied molecular orbital (LUMO) and thus energetic difference of the material (Eddy and Ita, 2011a-b). Firstly, at DFT within PBE and GW within G_0W_0 levels, we calculated the band structure, density of state (DOS) and partial density of state (PDOS) of perylene crystal using QUANTUM ESPRESSO (Giannozzi et al., 2009) and YAMBO (Marini *et al*., 2009) simulation packages. The electronic band structure plots along high-symmetry points Z→Γ→Ψ→A→B→Δ→E→X of the first Brillouin zone, setting Fermi energy level at 0 eV on the energy scale are presented in Figure 2. PBE exchange-correlation potentials are chosen over LDA because in several cases GGA-PBE gives more reliable and accurate results for DFT electronic properties calculation (Balesa, Lawal, Dalhatu, Idris, & Bello, 2021). For band structure calculations within PBE, the energy separation between the bottom of the conduction band and the top of valence band occurred at the Γ point, indicating that perylene is a direct band gap material with 1.3 eV energy gap, which is lower than the experimental value. However, to overcome the discrepancy from the DFT calculations (within GGA exchange-correlation potentials) and established experimental results, we further performed G_0W_0 calculation. It can be seen from the results that the inclusion of GW self-energy corrections, improve the the direct bandgap to 1.3 eV at Γ point calculated within GGA-PBE is corrected by bringing its value to 2.4 eV which is in good agreement with experimental value of 2.33-2.46 eV (Feng & Chen, 2005; Filapek, Matussek, Szlapa, Kula, & Pająk, 2016) as well. The calculated electronic band gaps of perylene crystal along with previous first-principles calculations and experimental data are presented in Table 1. Henceforth the fundamental band gap obtained with G_0W_0 agrees well with experimental results. Our calculation pointed out that G_0W_0 approximation on top of DFT provides an accurate prediction of the band structure. This energy gap value could be interesting for technological applications particulary solar cell.

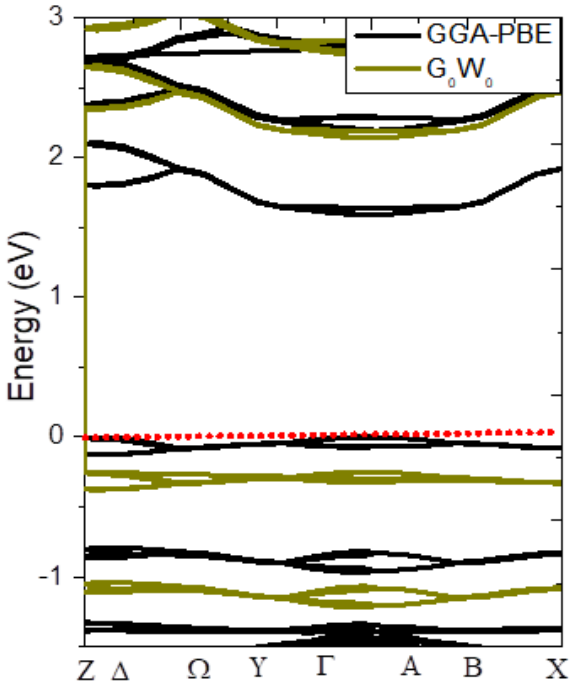

Fig. 3: Band structure of Perylene crystal

3.2 Optical properties of perylene

Generally, investigating optical properties plays a crucial role in understanding the optoelectronic behaviour of any material. From the comprehensive literature review, it is found that the exploration of the optical features relating to the perylene crystal is scarcely studied. To complete the study on the optoelectronic properties in addition to electronic properties, comprehensive studies are presented on the optical properties of the investigated compound by employing a method that give results in agreement with experimental measurement. In this paper, we have calculated the optical parameters using Yambo package and those based on on G_0W_0 approximation. The optical parameters investigated in this paper were real $\varepsilon_1(\omega)$ and imaginary$\varepsilon_2(\omega)$ parts of frequency-dependent

dielectric, reflectivity, refractive index, *n*, absorption coefficient, α and electron energy loss spectrum (EELS). The calculated optical parameters are shown in Figs. 3, 4 and 5. Fig. 3 shows the real and imaginary part of the frequency dependent dielectric function for perylene crystal. The real part of the dielectric function describes how much material has been polarized as a result of induced electric dipole creation by an external field, and the imaginary part defines how much material ability is for the absorption of photon energy. The obtained value for the real part of the dielectric function at 0 eV is $\varepsilon(0) = 4.92$. Conversely, this value is a significant parameter that could be also used to obtain the energy band gap value of perylene by Penn Model relation $\varepsilon_1(0) \approx \left(\hbar\omega_p/E_g\right)^2 + 1$ (Penn, 1962). Using plasma energy $\hbar\omega_p$ and the value of $\varepsilon_1(0)$, the value of energy gap of the title material can be calculated by using Penn expression. This value suggested that perylene crystal has huge potential to play the role as electron acceptor material due to the higher dielectric constant value which indirectly resulting to higher capability in conducting and transporting the electrons. The calculated $\varepsilon_2(\omega)$ with G_0W_0 show an absorption edge sometimes called optical gap at 2.4 eV, this value is related to QP band gap due to inter-band transition between conduction band minimum and valence band maximum states along $\Gamma\rightarrow\Gamma$ direction. The calculated optical gap is in good agreement with experimental value (Mizoguchi, Kano, & Wada, 2003; Zhou, Tajima, Yang, & Hashimoto, 2010). This point splits the conduction band maximum and valence band minimum (Lawal, Koma, & Godfrey, 2021; Lawal et al., 2017). The highest peak was observed at 2.91 eV indicating that perylene is a promising candidate for optoelectronic applications. The results of the imaginary part of the dielectric function indicated that perylene crystal has strong absorption behaviour in the visible light frequency, which depicts its suitability for solar cell applications.

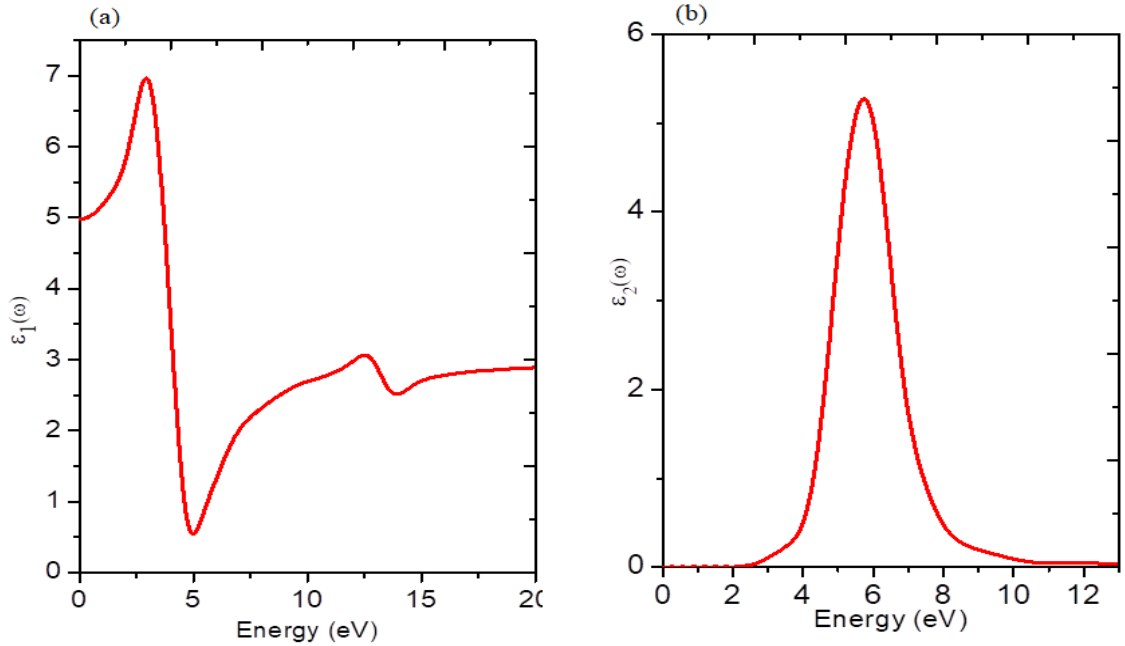

Fig. 3: Graph of (a) real part of dielectric function versus energy (b) imaginary part of dielectric function versus the energy of perylene crystal

Fig. 4 (a) and (b) show the energy dependence of absorption coefficient and refractive index. For photovoltaic applications, it is important to use a material with a suitable bandgap having a large absorption coefficient (Radzwan *et al*., 2020). When light rays strike the surface of a material, some part of its energy is reflected while some are transferred to the surface of the material. This transfer of energy to the surface is called Absorption of

light and it is represented in term of absorption coefficient α(ω). The graph for the variation of the absorption coefficient as a function of photon energy is presented in Fig. 3(a). From this graph, it is evident that perylene crystal has a good absorption coefficient in the visible light wavelengths. Since perylene crystal shows a good absorption coefficient in the visible light wavelengths, it is anticipated that the title material can be used as an absorbing layer for solar cell. The curves of refractive index n(ω) in Fig. 3 (b) is similar to the real part of the dielectric function $\varepsilon_1(\omega)$ which is in accordance with the established theory (Fox, 2002). The value of static refraction index was found to be 2.07.

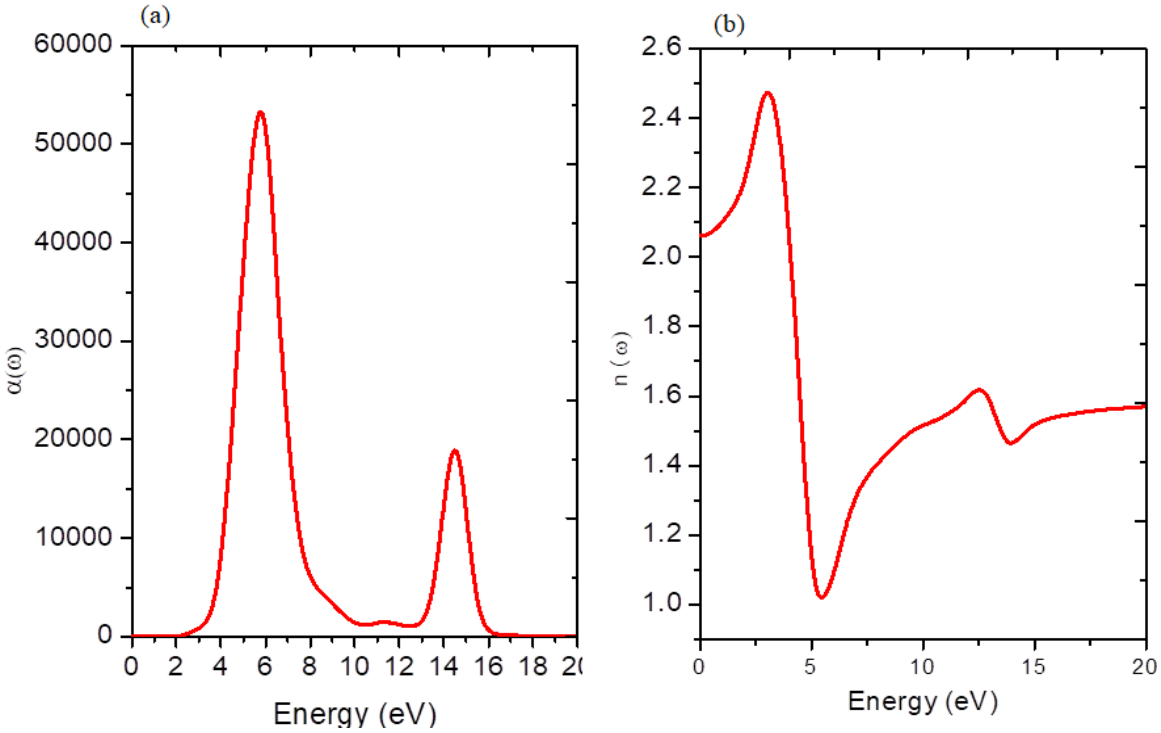

Fig. 4: Graphs of (a) absorption coefficient (b) refractive index, *n* of perylene crystal

Fig. 5 (a) and (b) show a graph of reflectivity and electron loss function (EEL) of perylene crystal**.** The reflectivity, $R(\omega)$ is one of the parameters that can be predicted from optical calculations. Reflectivity is the ratio of reflected photon energy from the surface to the photon energy incident on the surface (Shi, Pan, Zhang, & Yakobson, 2013). The reflectivity of perylene crystal is depicted in Fig. 5(a). Overall, the behavior of the reflectivity is maximum below 5 eV which makes the material suitable for applications in the visible and ultraviolet regions. The maximum reflectivity is due to the transitions among different energy bands. Reflectivity results reveal that perylene is mostly transmitted in the ultraviolet (UV) region because of small reflectance. Electron energy loss (EELs) functions is a tool that describes the loss in energy of a fast-moving electron in material from the top of a valence band to the bottom of a conduction band.. The energy loss function $-Im[1/\epsilon(\omega)]$ gives the energy loss of fast moving electrons in solids (Radzwan *et al*., 2020). The graph of energy loss function is represented in Figure 5(b). This graph gives us information about the loss in energy of the absorbed spectrum. The prominent peaks were found to be at 11.1. The sharp maxima peak in the energy loss function spectra represents the characteristics of plasma oscillations and this appears at a particular frequency called screened plasma frequency ω_P. At this point of energy, the real part of the dielectric function goes to zero indicating a rapid reduction in reflectance.

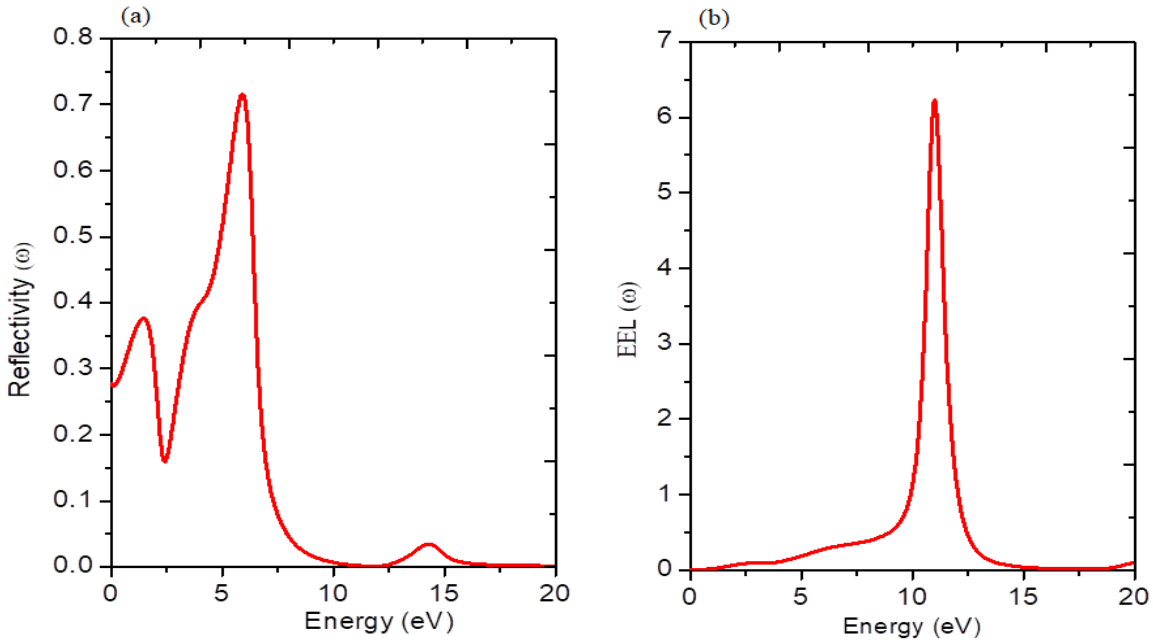

Fig. 4: Graphs of (a) reflectivity (b) Electron Loss function of perylene crystal

4.0 Conclusion

In conclusion, we have presented the structural, electronic and optical properties of perylene crystal. Highly accurate first-principles calculations as implemented in quantum Espresso and Yambo code were adopted. The calculated structural parameter with GGA-PBE exchange-correlation functionals are reasonably close to experimental results. The investigated electronic band structure reveals that perylene crystal is direct bandgap material. Our calculation pointed out that G_0W_0 approximation on top of DFT provides an accurate prediction of the band structure. We found the band gap value of perylene crystal with highly accurate method to be 2.4 eV and this value is consistent with experimental data. In addition to electronic properties, optical parameters are performed by evaluating frequency dependent dielectric function via random phase approximation (RPA) based on G_0W_0. Optical properties calculation show that the results attained with G_0W_0+RPA are in good agreement with available experimental measurement. Interestingly, optical gap of 2.4 eV and strong absorption of perylene in the visible light wavelength revealed that the material under investigation is suitable for solar cell applications. Hence, we have come to a conclusion that Perylene crystal is more compatible to serve as a new active material for applications in the OPV system.

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Not Applicable

Availability of data and materials

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Authors' contributions

This work was carried out in collaboration among all authors. Author Abdullahi Lawal and Musa Bello performed calculation of structural properties and sourced some relevant journals for the review. Authors Abdullahi Lawal and Ahmed Musa Kona performed calculations of optical properties. Author Abdullahi Lawal initiated the work. All authors took part in the compilation of results, proof reading and effecting all corrections. All authors read and approved the final manuscript.