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Quantum Mechanical Study of the Dielectric Response of V₂C-ZnO/PPy Ternary Nanocomposite for Energy Storage Application

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Abstract

With the proliferation of electronic gadgets and the internet of things comes a great need for lightweight, affordable, sustainable, and long-lasting power devices to combat the depletion of fossil fuel energy and the pollution produced by chemical energy storage. The use of high-energy-density polymer/ceramic composites is generating more curiosity for future technologies, and they require a high dielectric constant and breakdown strength. Electric percolation and Interface polarization are responsible for the high dielectric constant. To create composite dielectrics, high-conductivity ceramic particles are combined with polymers to improve the dielectric constant. In this work, ternary nanocomposites with better dielectric characteristics are created using a nanohybrid filler of V₂C Mxene-ZnO in a polypyrrole (PPy) matrix. Then, the bonding and the uneven charge distribution in the ceramic/ceramic contact area are investigated using quantum mechanical calculations. This non-uniform distribution of charges is intended to improve the ceramic/ceramic interface's dipole polarization (dielectric response). The interfacial chemical bond formation can also improve the hybrid filler's stability in terms of structure and, consequently, of the composite films. To comprehend the electron-transfer process, the density of state and electron localization function of the ceramic hybrid fillers are also studied. The polymer nanocomposite is suggested to provide a suitable dielectric response for energy storage applications.

Keywords Energy Storage · V₂C/ZnO hybrid · Polypyrrole · MXene · Nanocomposite

1 Introduction

A material's dielectric response measures how it reacts to an applied electric field. It is a basic property that governs several significant properties of a material, including its polarization, capacitance, and electrical conductivity. As it's crucial to the functionality of many devices and technologies, such as electronic components, energy storage devices, supercapacitors, solar cells, nanogenerators, and sensors, the dielectric response of a material is consequently of significant interest to the industry and academia [1]. In supercapacitors, a higher dielectric constant leads to a higher capacitance and energy density. In solar cells, a higher dielectric constant leads to a higher absorption of light and a higher efficiency. In nanogenerators and piezoelectric materials, a higher dielectric constant leads to a higher output voltage and power density. In sensors, a higher dielectric constant leads to a higher sensitivity and selectivity [2–5].

Polymer-based dielectric film are a type of energy storage device that has become important for advanced electronic

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devices and electric power systems [6–9]. As such, polymer nanocomposites [7–14], particularly those made from polypyrrole matrix reinforced with nanoscale fillers [11], are being researched for usage in dielectric applications. Flexible regenerated cellulose/polypyrrole composite films [15], polypyrrole/graphite composites [16], graphene/polypyrrole nanocomposites [17], Fe₃O₄-polypyrrole hybrid nanocomposites [18], BaTiO₃/polypyrrole nanocomposites [19], and poly(vinylidene fluoride) nanocomposites reinforced with polypyrrole-decorated graphene oxide are a few examples of polymer nanocomposites with improved dielectric properties [20]. These materials have exhibited high dielectric constants, low dielectric losses, and good stability, making them suitable for use in various dielectric applications.

For instance, in a study by Feng et al., the percolation threshold of poly(vinylidene fluoride-chlorotrifluoroethylene) (PVDF-CTFE) reinforced conducting poly(pyrrole) (PPy) nano-clips was reported to be about 7.4 wt % in all-organic nanocomposites [21]. Meanwhile, the dielectric constant of these nanocomposites was 23 times greater than that of the polymer matrix at 1 kHz and was lower than 0.4 over a wide frequency range. After being heated into a dielectric state, polypyrrole samples made with potassium persulfate or ferric chloride as oxidizing agents were observed to exhibit dielectric characteristics that were influenced by the quantities of the reactants employed in production [22].

In another study, polyvinyl alcohol (PVA), water-soluble polypyrrole (WPPy), and graphene oxide (GO) were combined to create flexible dielectric nanocomposites. The dielectric constant of these materials increased from 27.93 for an equal blend of WPPy/PVA to 155.18 for nanocomposites with 3 wt% GO loading, and the dielectric loss increased from 2.01 to 4.71 at 50 Hz and 150 °C [23].

Recent study showed that MXenes such as V₂C can be combined with several polymers for dielectric applications. PVC/MXene nanocomposites have been shown to have a high dielectric constant of 11,800 and low dielectric loss of 1.31 [24–26]. Poly(vinyl alcohol) (PVA)/V₂C MXene nanocomposite films have exhibited a permittivity of around 24 and a dielectric loss of around 0.14 at 1 kHz when using 4 wt% V₂C [27]. PVA/V₂C/cellulose have also been shown to have good dielectric properties, with a permittivity of around 21 and a dielectric loss of around 0.25 at 0.1 kHz when using 6 wt% MXene [28]. When using 2 wt% V₂C, it has been demonstrated that PVDF/La₂TiO₅/V₂C nanocomposites have a high dielectric constant of around 47 and a low dielectric loss of about 0.17 at 1 kHz [29]. Similarly, it was reported that V₂C MXene-SWCNT nanocomposites, when made with 5 wt % hybrid ceramic, have a high dielectric constant of around 232 and a low dielectric loss of about 0.2 at 0.1 kHz [30]. When employing 4 wt% V₂C, it has

been proven that polymer/V₂C/ionic liquid nanocomposites have a high dielectric constant of around 54 and a low dielectric loss of about 0.15 at 1 kHz [31].

Beside the use of PPy and V₂C-MXene based nanocomposite for dielectric applications, a well-known semiconductor material with a broad bandgap, excellent transparency, and strong chemical stability is zinc oxide (ZnO) which has also garnered great interest for dielectric application. ZnO nanocomposites have also been studied for their potential use in dielectric applications [32–35]. PVA/ZnO hybrid nanocomposite films [36], PVDF composites filled with core@double-shell structured Zn@ZnO@PS particles [37], and undoped and co-doped ZnO nanoparticles [32] are a few examples. These materials have shown improved dielectric permittivity, breakdown strength, and thermal conductivity, as well as suppressed dissipation factor and conductivity. They have potential applications in optoelectronic devices, high voltage insulation materials, and microwave devices. In addition, (PMMA/PVDF)/ZnO nanocomposites [38] have been shown to have good dielectric and mechanical properties, making them suitable for use in flexible electronics. Likewise, it has been shown that (PVA-PEO)-ZnO polymer nanocomposites [39] have enhanced dielectric performance and strong thermal stability.

A proposed hybrid material with improved electrical conductivity, dielectric characteristics, and transparency is possible when PPy/V₂C MXene and ZnO are combined. Therefore, given the importance of the dielectric response in materials science and the potential applications of PPy/V₂C MXene-ZnO, it is crucial to investigate the dielectric response of this material in order to understand its properties and optimize its performance. In this study, we use first-principles calculations to investigate the dielectric behaviour of PPy/V₂C MXene-ZnO, with the aim of understanding the underlying mechanisms in the ceramic hybrid fillers and predicting its potential applications. The ternary composites exhibit a well-maintained high electrical breakdown strength, according to the electron localization function (ELF) results. Besides, due to the decreased hole quantity of the point charge in the Zn-V dipole, the charge transfer analysis suggests that an increase in the charge quantity at Zn may signify an improved dielectric response in ternary composites. It is notable that adding ZnO to V₂C resulted in a greater contribution of V₂C electrons to the Fermi level, as shown by the density of states (DOS) study.

2 Computational Method

In this study, we used first-principles calculations to investigate the dielectric response of PPy/V₂C MXene-ZnO. For our calculations, we used the density functional theory

(DFT) method, which is a widely used and well-established first-principles calculation method [40–48]. DFT is based on the idea that through the self-consistent solution of the Kohn-Sham equations, the total energy of a system may be represented as a function of the electron density. In our calculations, we used the exchange-correlation functionals to describe the electron-electron interactions within the material. The Exchange-correlation functional is approximately modelled using generalized gradient approximation (GGA) and Perdew – Burke – Ernzerh (PBE). First, the structure of the V_2C -MXene was modelled with 3×3 periodic supercell lattice structure having a , b , & γ of 8.68 Å, 8.68 Å, and 120° , respectively. The adoption of a vacuum space of about 15 Å perpendicular to the lattice plane prevented interactions between repeated pictures. Similarly, the ZnO structure was also modelled with 2×2 non-periodic supercell. We then performed structural optimization to relax the positions of the atoms and minimize the total energy of the system by using DMol³ in Materials Studio software. 1×10^{-6} eV was the Self Consistent Field (SCF) tolerance used for the optimization. Once the optimized structures were obtained, we performed adsorption calculation using Adsorption Locator calculator in Materials Studio to generate the most stable and optimized V_2C Mxene-ZnO configurations. Thereafter, a series of calculations to determine the energetics and electronic properties of V_2C Mxene-ZnO was conducted using Cambridge Sequential Total Energy Package (CASTEP). For these calculations, 571 eV was employed for the plane wave cutoff energy, and the Brillouin zone of $10 \times 10 \times 1$ k-points was used. Long-range van der Waals interactions are taken into account using Tkatchenko-Scheffler method for the DFT dispersion correction [49]. Whereas OTFG ultrasoft with Koelling-Harmon were employed for the pseudopotential and relativistic treatment.

3 Results and Discussion

DFT calculations were used to determine the charge distribution in the optimized structural unit of ZnO and V_2C -MXene in order to examine the dielectric mechanism in the ceramic hybrid filler (Fig. 1a & b). Mulliken population analysis establishes the appropriate values of charges. Meanwhile, some of the Zn atoms in the ZnO are adsorbed onto the V_2C surface, as shown by Fig. 2. This figure presents the schematic 3D diagram of the ZnO/ V_2C interface with the optimum geometric structure. After hybridization, V atoms from the surface of V_2C may interact with Zn atoms from the surface of ZnO to produce Zn-V metallic bonds. At the V_2C /ZnO contact area, the average ZnV bond length is 2.62 Å. And the values in red represent the precise charge transfer values as established by the Mulliken population study.

Due to the lower hole amount of the point charge in the Zn-V dipole, an increase in the charge quantity at Zn may indicate an enhanced dielectric response in ternary composites. The hybrid filler's interface zone has a non-uniform distribution of charges due to the chemical bond that exists there. Such an uneven distribution of charges can improve the ceramic/ceramic interface's dipole polarization which is the dielectric response [48]. Interfacial chemical bond formation can also improve the structural stability of the hybrid filler and, consequently, of the composite films. Ultimately, the semiconducting ZnO ceramic filler's dielectric responsiveness is enhanced by the development of a V_2C -ZnO hybrid structure.

The DOS diagram for the s, p, and d-orbital electrons in the V_2C /ZnO structure is shown in Fig. 3a. At the Fermi level, the d orbital electron distribution was more prevalent. Similarly, the p-orbital electron distribution was equally very prevalent at the Fermi level. The contribution of the Fermi-level electrons might therefore be improved by increasing the amount of d and p orbital electrons. The density of states (DOS) values for the V_2C and V_2C /ZnO structures are displayed in Fig. 3b. The DOS diagram in this

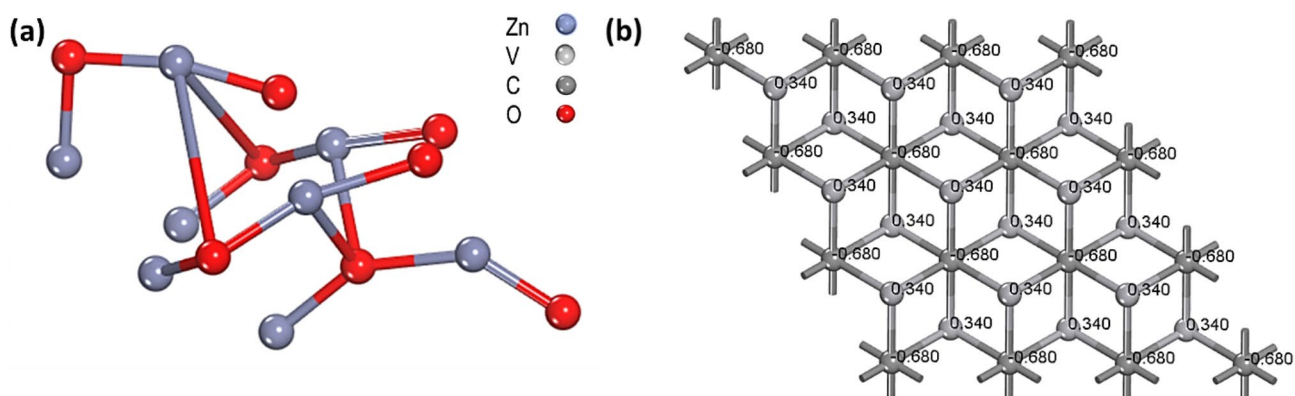


Fig. 1 (a) 3D structural representation of optimized ZnO, (b) Top-surface of the structural representation of V_2C -MXene

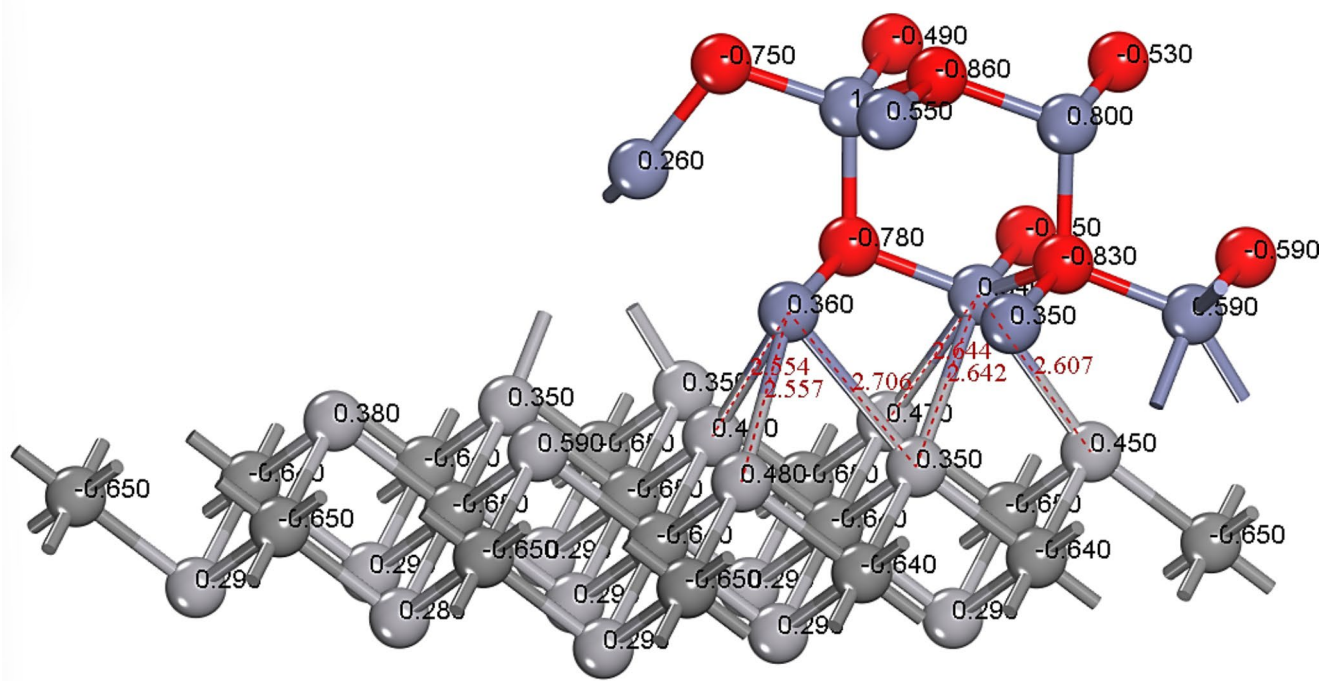


Fig. 2 Optimized 3D structural configuration of V_2C/ZnO hybrid with charge distribution

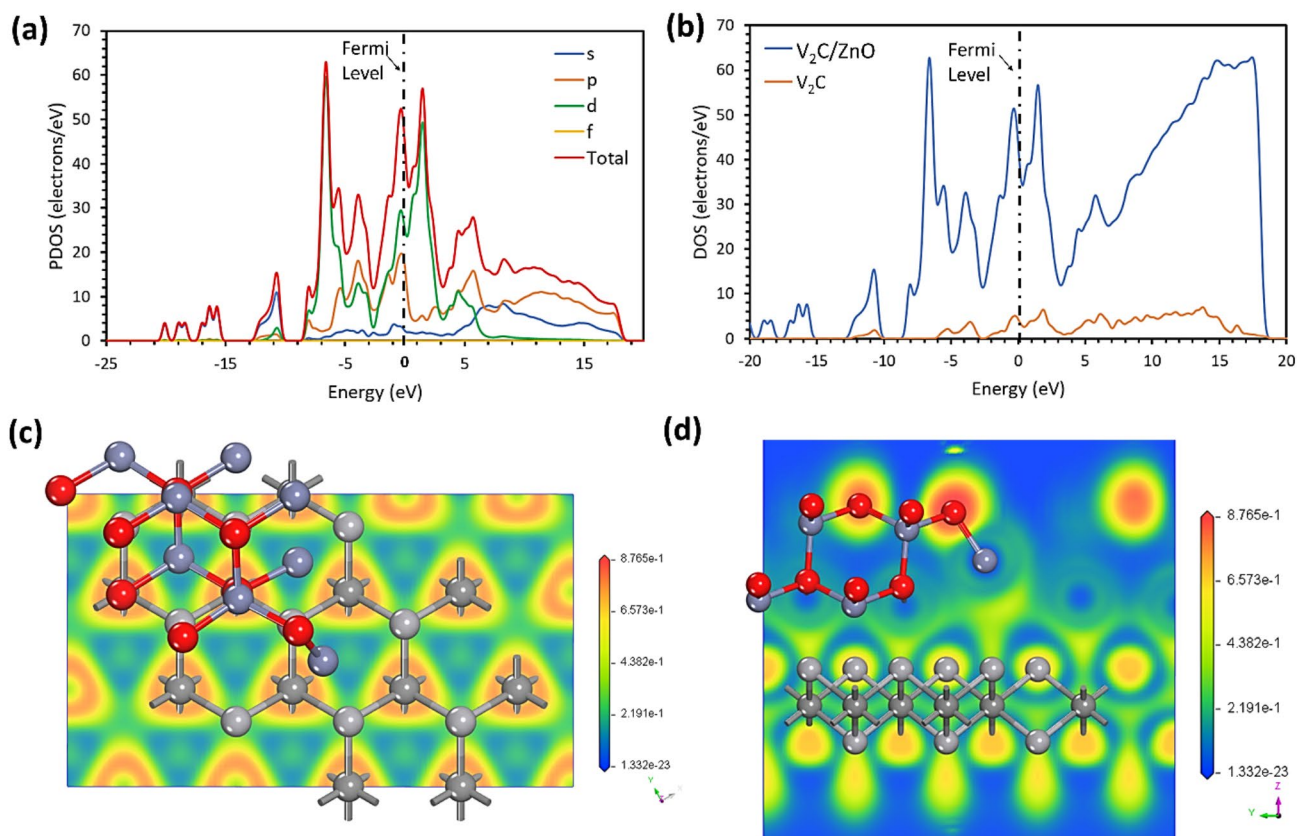


Fig. 3 (a) The DOS diagrams for the s, p, and d-orbital atoms in the V_2C-ZnO , (b) The results of the DOS of the atoms for the structure (c), The top-surface ELF result, and (d) The side-surface ELF result

instance is produced by superimposing the results of the total DOS of V_2C before and after hybridization with ZnO. It is interesting to note that adding ZnO to V_2C exhibited increased Fermi level contribution from V_2C electrons.

Becke and Edgecombe established the electron localization function (ELF) as a “simple measure of electron localization in atomic/molecular systems.” [50] The ELF of the V_2C/ZnO structure was determined to further elucidate the electron localization contribution of the valence-band electrons at the surface. The ELF findings for the top and side surfaces of the V_2C/ZnO were shown in Fig. 3c and d, respectively. Yellow and orange, which represent the localisation of electrons in atomic systems on the ELF map, were displayed [44]. The electron localization map showed enhanced electron localization in ZnO which led to the increased electron movement in the of the V_2C/ZnO structure. And this is in line with the DOS for the V_2C and V_2C/ZnO structures.

In sum, the compact V_2C/ZnO interface created by the bonding method prevented an increase in the leakage conduction at the V_2C/ZnO interface. Results indicate that the ternary composites have a well-maintained high electrical breakdown strength. As a result, the electrical characteristics of the ternary composite films for possible energy storage applications could be perfectly balanced as desired.

4 Conclusion

In this study, we used first-principles calculations to investigate the dielectric response of the ceramic-ceramic interface in PPy/ V_2C -ZnO ternary composite. The results of our calculations showed that the V_2C -ZnO ceramic-ceramic contact area display a strong dielectric response. This suggest that PPy/ V_2C -ZnO may have potential applications in energy storage, electronics, and optoelectronics, where the dielectric response is an important factor. In addition, the results of the electron localization function (ELF) test show that the electrical breakdown strength of the ternary composites is well-maintained and high. Moreover, according to the Mulliken charge transfer study, a rise in the charge quantity at Zn may signify an improved dielectric response in ternary composites because the point charge in the Zn-V dipole has less hole content. It is interesting to note that the density of states (DOS) study showed that the contribution of V_2C electrons to the Fermi level increased when ZnO was added to V_2C . This property explains the ability of the material to exhibit electron mobility for an enhanced dielectric response. Overall, our study provides a comprehensive analysis of the dielectric response of V_2C/ZnO hybrid interface and offers new insights into the underlying mechanisms that govern its properties. These results contribute to a better

understanding of this new class of materials and can help to guide the design and optimization of PPy/ V_2C -ZnO -based devices and technologies.

There are several directions for future work that could build upon the results of this study. For example, it would be interesting to investigate the frequency dependent dielectric response and the effect of different factors, such as composition, temperature, and strain, on the dielectric response of PPy/ V_2C -ZnO. The application of PPy/ V_2C -ZnO in various device designs and applications, such as supercapacitors, touch screens, solar cells, and sensors, would also be worthwhile to investigate. A high dielectric constant and low loss tangent can lead to improved performance in high-frequency applications and its ability to be used as a conductive layer or sensing material will make it a promising material for various device designs and applications. Further research in these areas could help to fully realize the potential of PPy/ V_2C -ZnO as a promising new class of materials.

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Data Availability Data availability is on request.

Declarations

Conflict of interest The authors declare no conflict of interest.

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