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Investigation of the Dielectric Response of PPy/V_2C MXene – ZnO using Quantum Mechanical Calculations

By:

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CONFERENCE ON NANOMATERIALS

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Outline

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Background

Polymer-based dielectric film

Polymer-based dielectric film are a type of energy storage device that has become important for advanced electronic devices and electric power systems.

(Li et al., 2021)

Dielectric materials are used to separate and insulate conductive materials from each other, such as in capacitors, transistors, and other electronic components.

Polymer-based dielectric films are used in a variety of electronic applications, such as in capacitors, flexible printed circuit boards, and flat panel displays. They are also used in energy storage devices, such as batteries and supercapacitors.

Kim, 2022

Background

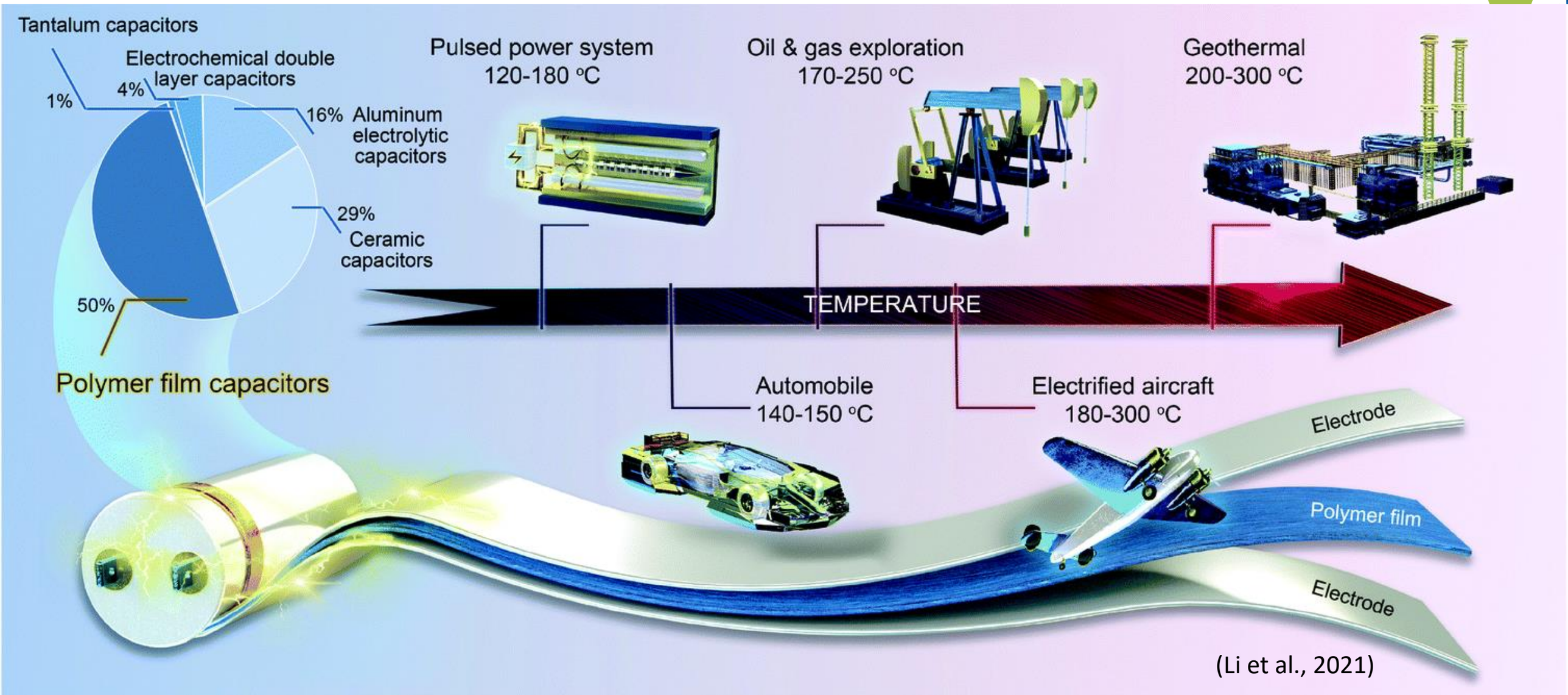


Figure 1: Applications of high-temperature dielectric polymer film capacitors and market share of the world's high-voltage capacitors

Background

ZnO

Zinc oxide (ZnO) is a well-known dielectric material with excellent electrical properties, making it a promising candidate for energy storage applications. Dielectric materials like ZnO can store electrical charge through polarization of their internal electric field, making them useful for capacitive energy storage.

Deng, 2021, Feng, 2021

Production: ZnO can be synthesized through a variety of techniques, including chemical vapor deposition, sol-gel, and hydrothermal methods, making it possible to produce high-quality ZnO films with tailored properties.

Deng, 2021

Properties: ZnO is a wide-bandgap semiconductor, which means it has a large energy gap between its valence and conduction bands. This property makes it an excellent candidate for use in high-temperature and high-power electronic devices, including energy storage devices.

Deng, 2021

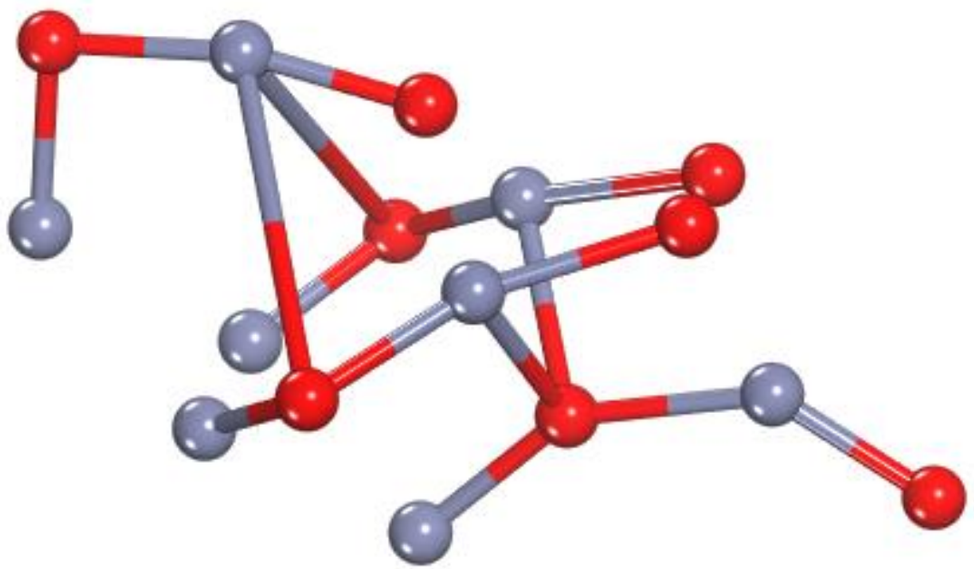


Figure 2: An illustrative of the 3D chemical structure of ZnO.

Background

V2C-MXene

V2C MXene is a two-dimensional transition metal carbide with excellent electrical and mechanical properties, which make it a promising candidate for various energy storage applications, including dielectric energy storage.

Yao, 2022, Mohammed, 2022

Properties: V_2C MXene has high thermal stability, excellent mechanical strength, and can be synthesized in large quantities through a scalable process.

Mohammed, 2022

Applications: V_2C MXene a promising candidate for various energy storage applications, including high-energy-density capacitors, electrochemical capacitors, and other dielectric energy storage devices.

Yao, 2022,

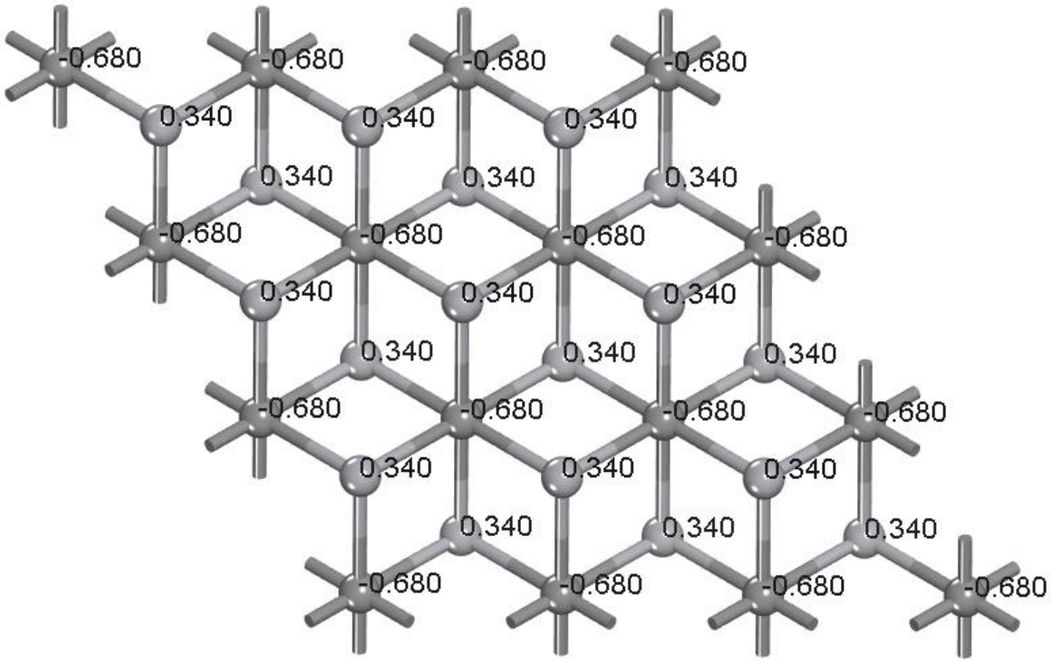


Figure 3: An illustration of V_2C MXene material.

Introduction

DFT **Density Functional Theory**- First principle / Ab-initio / Quantum mechanical Calculation

MC **Monte Carlo** classical calculation

Adsorption Locator identifies possible adsorption configurations by carrying out Monte Carlo searches of the configurational space of the substrate-adsorbate system as the temperature is slowly decreased.

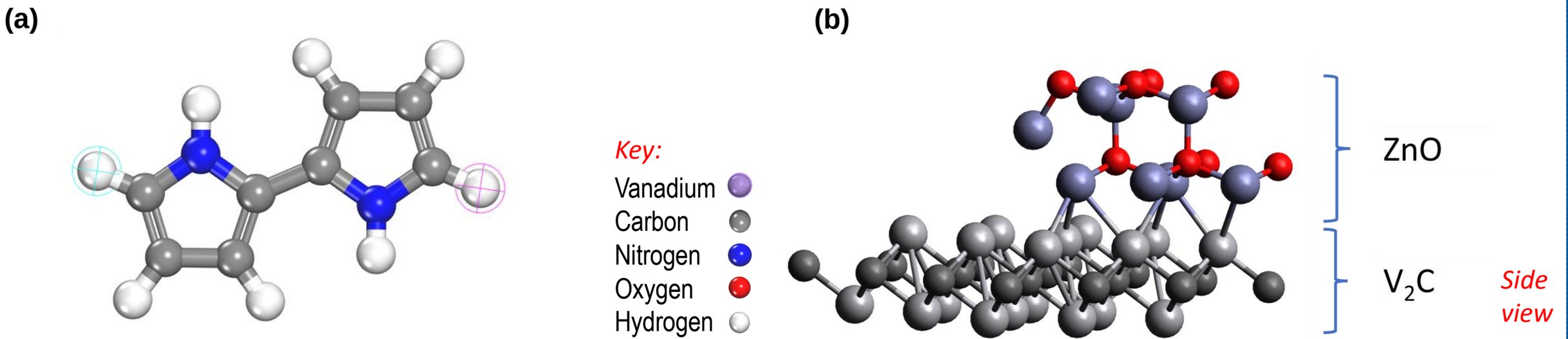
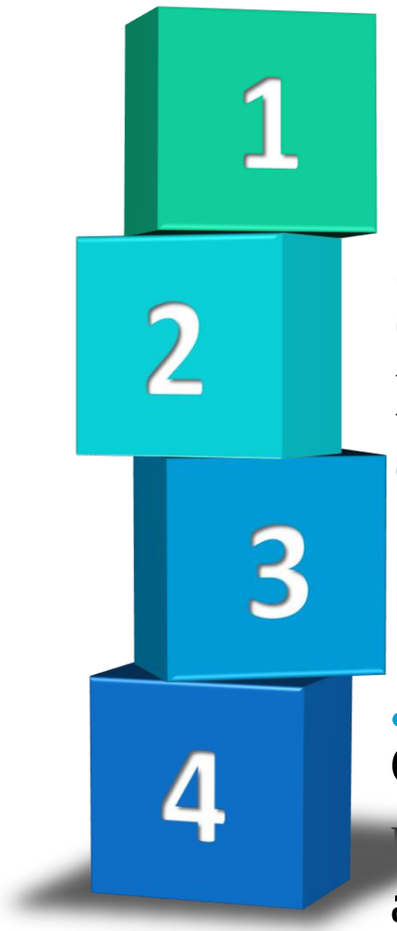


Figure 4: (a) PPy molecule and (b) ZnO-V2C MXene hybrid.

Research Goals

Study the molecular interaction of V_2C with ZnO using Density Functional Theory (DFT) and Monte Carl (MC).

Analyze the resulting charge distribution and electronic properties.



Obtain insight into the electron localization function of the ceramic-ceramic systems.

Conclude on the suitability of the nanocomposite for dielectric application.

Methodology

Computational procedure

Builder	01	Molecular Model Development	▪ Construction of the PPy molecule, ZnO, and MXene structure were done with polymer and crystal builder.°.
DFT	03	Geometry Optimization/Equilibration	Relaxing and optimizing the structures of the system to minimize the energy of the system.
Monte Carlo	03	Adsorption Locator and Annealing	100,000 loading steps at 10 heating cycles with 50,000 steps per cycle. The energy window and maximum adsorption distance chosen were 100Kcal/mol and 10A
DFT	04	Energy Calculation: Structural and electronic	Simulate the electronic properties using plane wave DFT
	05	Functional and Basis set	A generalized gradient approximation (GGA) functionals, coupled with by Perdew, Burke, and Ernzerhof (PBE) scheme
	06	Post-processing /Analysis	Elucidation of properties from simulation output

Results and Discussion

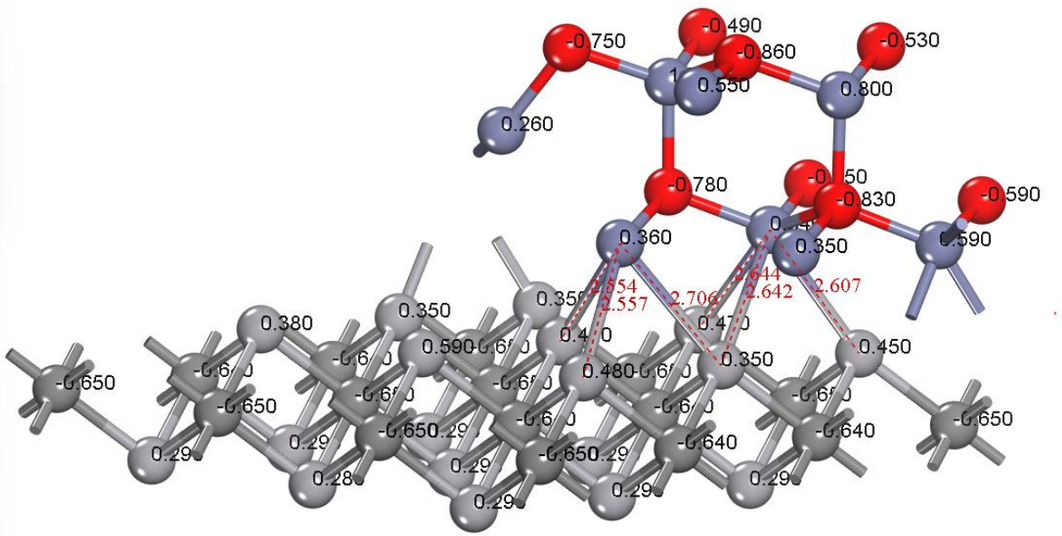
Adsorption Analysis

$$P_{mn} = min\left(1, \frac{\rho_n}{\rho_m}\right)$$ ---------- equation 1

Where ρ_m is the frequency of sampled m configurations, ρ_n is frequency of proposed n configurations and P_{mn} is the probability of transition of configuration from m to n.

$$E_{ads} = E_{V2C_+ZnO} - (E_{V2C} + E_{ZnO})$$ ---------- equation 2

Where E_{ads} is the adsorption energy of ZnO on V_2C.
E_{V2C_+ZnO} is the total energy of the ZnO - V_2C system, and E_{V2C} and E_{ZnO} are the single point energies of the sorbate and substrate



Adsorption distance: At the V_2C/ZnO contact area, the average ZnV bond length is 2.62 Å.

Figure 5: Optimized 3D structural configuration of V_2C/ZnO hybrid with charge distribution

Results and Discussion

Charge transfer (Electron Density Difference)

$$\Delta\rho = \rho_{V2C_+ZnO} - (\rho_{V2C} + \rho_{ZnO}) \quad \text{---------} \quad \text{equation 4}$$

where $\Delta\rho$ is the charge density difference

ρ_{V2C_+ZnO} is the electron density of the total $host$+Na system, and

ρ_{V2C} and ρ_{ZnO} are the unperturbed electron densities of the substrate (V_2C) and sorbate (ZnO), respectively.

The isosurface value is ± 0.01e/Å^3

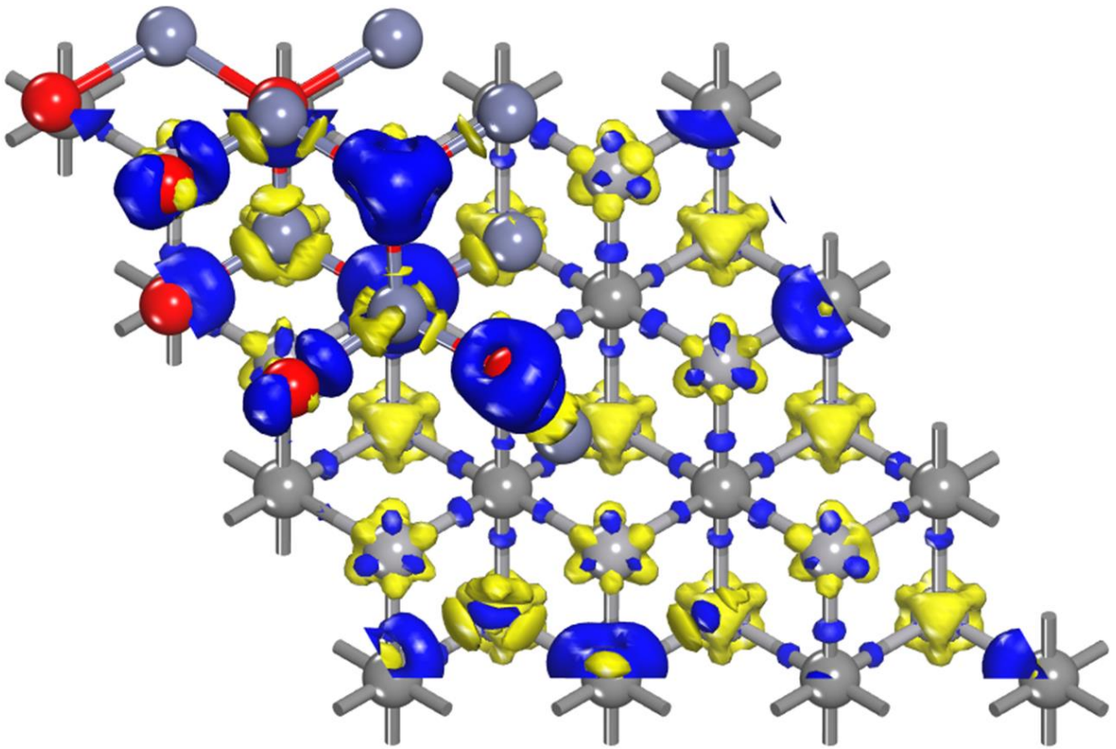


Figure 6: Electron density difference of V_2C/ZnO hybrid

The yellow region denotes depletion of charge density, while the blue region represents charge density accumulation

Electronic analysis

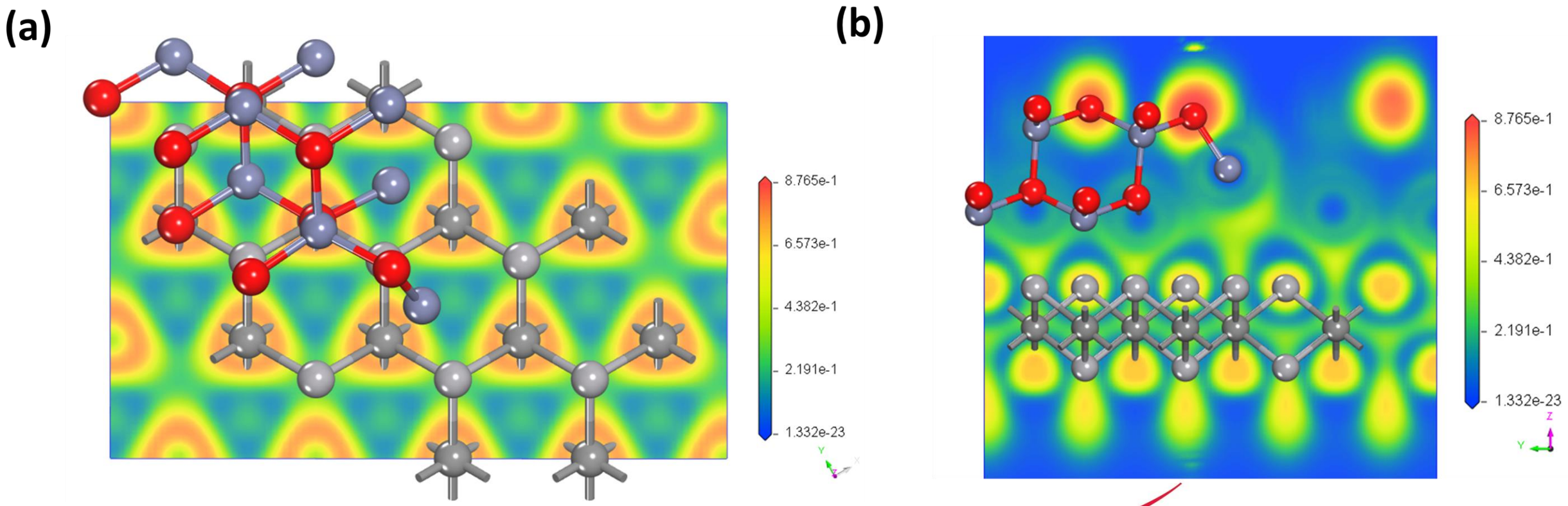


Figure 7:(a), The top-surface ELF result, and (b) The side-surface ELF result

Electronic analysis

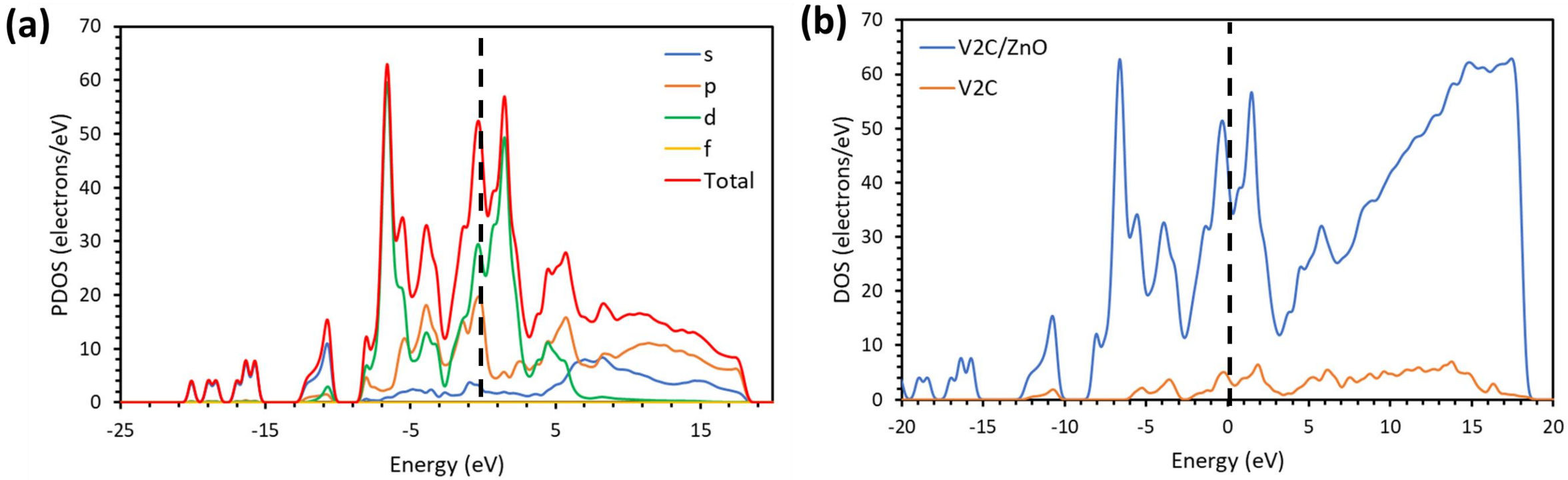


Figure 8: (a) The DOS diagrams for the s, p, and d-orbital atoms in the V2C-ZnO, (b) The results of the DOS of the atoms for the structure

The nanocomposite is semi-conductive, many of the states arise from each type of orbital, s, p, or d

Conclusion

we used first-principles calculations to investigate the dielectric response of the ceramic-ceramic interface in PPy/V2C-ZnO ternary composite.

1. V2C-ZnO ceramic-ceramic contact area display a strong dielectric response.
2. Charge transfer study, a rise in the charge quantity at Zn may signify an improved dielectric response
3. DOS study showed that the contribution of V2C electrons to the Fermi level increased when ZnO was added to V2C.
4. the electron localization function (ELF) test show that the electrical breakdown strength of the ternary composites is well-maintained and high.
5. It would be interesting to investigate the frequency dependent dielectric response and the effect of different factors

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Thank you for listening