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Investigation of the Dielectric Response of Ppy/V_2c Mxene-Zns from First Principle Calculation

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Abstract : High-energy-density polymer/ceramic composites require a high breakdown strength and dielectric constant. Interface polarization and electric percolation are responsible for the high dielectric constant. In order to create composite dielectrics, high conductivity ceramic particles are combined with polymers to increase the dielectric constant. In this study, bonding and the non-uniform distribution of charges in the ceramic/ceramic interface zone are investigated using density functional theory (DFT) modeling. 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 structural stability of the hybrid filler and, consequently, of the composite films. To comprehend the electron-transfer process, the density of state and electron localization function of the PPy with hybrid fillers are also studied. The polymer nanocomposite is anticipated to provide a suitable dielectric response for energy storage applications.

Keywords : energy storage, V_2C/ ZnS hybrid, polypyrrole, MXene, nanocomposite, dielectric
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