DFT Modeling and Impedance Spectroscopy Analysis of a High Performance Zirconia-Based Solar Cell

The development of modern technologies requires a balanced approach that considers both environmental sustainability and economic feasibility. The large-scale adoption of silicon-based solar cells remains limited due to high production costs and environmental challenges. Herein, we present a chalcogenide-based solar cell of the configuration, FTO/SnO_2/$SrZrS_3$/Cu-MOF/C, made of affordable materials. The cell reports a theoretical power conversion efficiency of 32.28%. The simulation was carried out using SCAPS-1D device simulator, whereas the optical parameters were determined using the density functional theory (DFT). The device exhibits an open-circuit voltage (V_{oc}) of 1.10 V, a short-circuit current density (J_{sc}) of 35.89 mA/cm^2, and a fill factor (FF) of 82.20%. The absorption coefficient (α) of the perovskite compound, $SrZrS_3$, was found to increase with low-energy absorption, reaching its first peak at 13.74 eV with a magnitude of 2.44×10^5 cm^{-1}. Further, the relative permittivity of the materials used in this work was measured using impedance spectroscopy analysis. It was found that high permittivity improves the cell's tolerance to various non-idealities, particularly in the early stages of device development when the structure is optimized.