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Density functional theory study of cobalt sulfide as a counter electrode material for dye-sensitized solar cells

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Dye-sensitized solar cells (DSSCs) are viewed as potential substitutes for traditional silicon-based solar cells due to their affordability, impressive performance in low-light conditions, eco-friendly energy production, and adaptability in solar product integration. The use of noble metals such as platinum as counter electrodes in DSSCs was initially limited by their high cost; however, cobalt sulfide (CoS) has been recognized as a viable alternative due to its abundance, non-toxic properties, and cost-effectiveness. In this work, the crystal structure, electronic, optical characteristics, and electrocatalytic activity of the tetragonal phases of cobalt sulfide are investigated through density functional theory with a quantum espresso (QE) package. The results obtained for the lattice parameter are a = b = 3.53 Å and c = 4.80 Å. The generalized gradient approximation and hybrid exchange-correlation function yield bandgaps of 1.63 and 1.69 eV, respectively, which are consistent with the reported experimental values. An analysis of the density of states and the projected density was carried out to validate the accuracy of the calculated band gaps. Additionally, significant information was obtained from the optical properties through the calculation of the dielectric function. The findings reveal real and imaginary static dielectric constants of 11.85 and 0.13, respectively. Furthermore, the measured absorption and conductivity spectra exhibit promising attributes in the UV–visible range and good electrical conductivity. Moreover, the electrolytic activity was studied to analyze the adsorption energy of CoS and the electrolyte. Generally, the calculated electronic and optical properties of CoS crystals indicate their potential application as CEs in DSSCs.

Abstract Category

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