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Computational insights into the bulk and surface properties of cobaltite: A combined DFT-D+U and atomistic simulation study

Cobaltite (CoAsS) possesses a similar structure to that of pyrite (FeS₂), exhibiting a semiconducting behaviour. Its X-ray diffraction pattern has been shown to closely resemble that of FeS₂ with the cleavage occurring along (100), (021), (111) and (110) planes in order of decreasing prominence. Cobaltite is commonly found in a variety of ore deposits, particularly in high temperature veins or in metamorphosed rocks. The mineral undergoes oxidation when exposed to oxygen and water producing a solution containing acid and heavy metals; therefore, understanding its surface stability is crucial for the extraction of valuable minerals. The density functional theory with dispersion correction and U parameter (DFT-D+U) and atomistic simulation with novel potentials were employed to correctly predict the bulk and surface properties of cobaltite. It was found that the d-orbital of cobalt (Co) with U = 1.0 eV was optimum to correctly predict a band gap of 0.589 eV for the bulk cobaltite model. The interatomic potentials used in atomistic simulations were able to predict lattice parameters of a = b = c = 5.543 Å, which correlate very well with the DFT-D+U value of 5.549 Å. The DFT-D+U calculations indicate that the surface stability in cobaltite follows the order (100) > (021) in decreasing rank, suggesting that the (100) surface is the most stable. This trend is corroborated by atomistic simulations results, which also show that the surface energy of (100) is lower than that of (021), further confirming its stability. This study showed the consistency between the DFT-D+U and atomistic simulations, providing insights into the surface stability that offer a fundamental understanding of the cleavage of cobaltite during mineral processing.

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