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Theoretical Insights into Mooihoekite: A DFT-D Investigation of the bulk properties.

Mooihoekite (Cu₉Fe₉S₁₆) is a copper-iron sulfide mineral belonging to the chalcopyrite derivative family, characterized by its metal-enriched composition. It crystallizes in the tetragonal system and is commonly found in association with minerals such as haycockite, magnetite, pentlandite, mackinawite, and sphalerite. Despite its structural similarity to the well-studied chalcopyrite, Mooihoekite remains relatively underexplored from both computational and experimental perspectives. To address this gap, this study employs density functional theory with dispersion corrections (DFT-D) to investigate the bulk properties of Mooihoekite. The Hubbard U parameter is incorporated to account for correlation effects arising from localized d-states on transition metal atoms. The calculated structural parameters and interatomic distances show excellent agreement with available experimental data. Electronic structure analysis reveals semiconducting behavior with a band gap of approximately 0.7 eV and antiferromagnetic ordering, evidenced by predominantly symmetric spin-up and spin-down density of states (DOS). Mechanical stability is confirmed through the calculated elastic constants, which satisfy all stability criteria, while the Pugh ratio (B/G) indicates ductile behavior. The ground-state magnetic moment is determined to be ~5 μB at 0 K, consistent with experimental observations of temperature-dependent magnetism. These findings provide a foundational understanding of Mooihoekite's structural, electronic, mechanical, and magnetic properties, paving the way for further exploration of its surface chemistry and potential applications.

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