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# Study of the electronic, bonding, elastic and acoustic properties of covellite via first principles

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**Abstract:** Covellite (CuS) is a compound with a simple chemical formula but a rather complex crystal structure. In this work, we studied the electronic, bonding, elastic and acoustic properties of covellite by first principles calculation. Electronic property calculations reveal that the p-d hybridization between S-3p and Cu-3d is responsible for the metallic behavior of covellite, which makes it a challenge to construct an accurate ionic model for this compound. The calculated partial density of states reproduce the experimental XPS and XAS well and the theoretically obtained Fermi surface verifies the experimentally found two-dimensional electronic transport characteristic of covellite. Calculated elastic constants demonstrate that covellite is mechanically stable but anisotropic. Investigation reveals that elastic constant  $C_{44}$  has a close correlation with the easy-cracked property of  $c$  axis of covellite. Besides, bulk modulus, shear modulus, Poisson's ratio, velocities of acoustic waves and Debye temperature were also predicated. Proceeding from the Christoffel equation of hexagonal crystal, we also discussed the propagation properties of acoustic waves in covellite to give a theoretical guidance for the related measurement.

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