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First-principles studies of electronic, transport and bulk properties of pyrite FeS[1] DIPENDRA BANJARA, AUGUSTINE MBOLLE, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We present results of ab-initio, self-consistent density functional theory (DFT) calculations of electronic, transport, and bulk properties of pyrite FeS_2. We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) formalism, following the Bagayoko, Zhao and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). The BZW-EF method requires successive, self consistent calculations with increasing basis sets to reach the ground state of the system under study. We report the band structure, the band gap, total and partial densities of states, effective masses, and the bulk modulus.

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