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Magnetic states and high-pressure enthalpy landscape of manganese sulfide polymorphs: a first-principles study

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We combine density functional theory (DFT) with special quasirandom structures (QRS) and occupation control matrix (OCM) methods to investigate the magnetic ordering and pressure effects on manganese sulfide polymorphs. MnS is usually found in paramagnetic (PM) rock-salt (RS) structure under ambient conditions, but it becomes antiferromagnetic (AFM) as temperature decreases at constant pressure. On the other hand, at room temperature, it has been observed that MnS undergoes pressure induced structural transformations. Our study shows that by taking into account the ordering/disordering of the local magnetic moments and the explicit control of the Mn ⊠-electrons' localization, the computed energy bandgaps and local magnetic moments are in excellent agreement with those reported experimentally, particularly for PM-MnS.
Finally, by studying the enthalpy landscape of various MnS polymorphs, we identify at about 21 GPa, the structural transformation from RS to orthorhombic MnP-type. This structural transformation seems to explain previously reported experimental results of a new stable but unidentified MnS phase at similar pressure.

Category

Solid State (Theory)

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