THE LOSS OF MAGNETISM IN FeS UNDER HIGH PRESSURES

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We argue that the formation of the non-magnetic state of FeS in external pressures above 6.5 GPa is in agreement with the prediction of the quantum atomistic solid-state theory (QUASST), an extension of the crystal-field theory with the spin-orbit coupling incorporated, and is related to the change of sign of the off-cubic trigonal distortion marked by the change of the c/a ratio from > 1.63 (magnetic) to < 1.63 (non-magnetic). In the calculations we take into account very strong correlations among six d electrons within the incomplete $3d$ shell, the crystal field, relativistic spin-orbit coupling and two Hund's rules. Our QUASST approach allows to calculate both zero-temperature properties and whole thermodynamics.

9.7 cm

13.4 cm

Subject category :

3. Transition Metals, Alloys and Compounds

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