Crystal, Magnetic and Electronic Structure of the Pentlandite Series

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The mineral Pentlandite (Pn) is one of the most economically important minerals in magmatic Ni-Cu-platinum group element (PGE) deposits, and typically occurs on Earth with a composition around Fe/(Fe+Ni) ~ 0.5 [1,2]. Pn is also an important component in extraterrestrial rocks, which however occurs with a composition Fe/(Fe+Ni) ~ 0.7 [3,4]. The existence of this compositional variability has remained enigmatic. We have performed ab-initio calculations on the (Fe,Ni)-Pn series. The structures obtained using the special quasirandom method are discussed with applications to mineral formation in terrestrial vs extraterrestrial environments. Our results shed light on the effectiveness of computational approaches for disordered-highly correlated systems.

The results have broader implications on the prediction of the mineralogy of planetary interiors. Volume, density and elemental partitioning changes in minerals have been observed experimentaly to coincide with pressure-induced mineral spin-transitions, suggesting that exchange interactions may be important for driving the variability of mineral compositions (5,6). However, it is not possible to experimentaly confirm the existance of this mechanism, as the composition and spin transitions may also be independantly induced by compression or may have a correlated, but not causal relation. Our calculations on Pn confirm the existance of this mechanism, by showing that the optimal ambient-pressure mineral composition minimizes a quantity which is proportional to magnetization. We discuss a rationalization for the existance of this mechanism. The result stresses the importance of characterizing mineral spin-transitions for the purposes of mapping the mineralogy of planetary interiors.

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