

## **Evaluating the physicochemical conditions for gold occurrences in pyrite**

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### **ABSTRACT**

While noble metals often occur as minor components in host minerals in various ore deposits, little theoretical assessment exists to predict the occurrence of these metals. Here, we probe the fundamental controls responsible for the occurrence of trace elements in host minerals through first-principles calculations. We apply the theoretical model to understanding the debated issues concerning the occurrence of gold (Au) in pyrite, in which the valence of Au is ascribed to either positive or negative values. Our results indicate that (1) both positive and negative valent Au may occur in pyrite and (2) higher sulfur fugacity and lower temperature lead to more Au<sup>+</sup> occupying Fe sites in pyrite. These findings suggest that chemical states and speciation of the Au in host pyrite are ultimately controlled by temperature and sulfur fugacity, providing insight into the formation conditions of ore deposits and facilitating strategy design for beneficiation.

**Keywords:** Gold-bearing pyrite, physicochemical condition dependence, gold occurrence, density functional theory, thermodynamics, sulfur fugacity