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# Simulation study of Au occurrence state in arsenopyrite crystal

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Arsenopyrite often contains significant quantities of Au, and it is thus important to study its distribution controls. Au in arsenopyrite was investigated by Density Functional Theory (DFT) calculations, focussing on electronic and structural details. Energetically, Au substitutes for S (-2.73eV) or As (-2.97eV). Hirshfeld analysis showed that Au occurred as $Au^0$ in arsenopyrite by substituting for S or As atom for the electrons to drift to Fe or As. There were no anti-bond behaviour in ideal arsenopyrite crystals, but when the Au substituted for S, the anti-bonds of As-Au appeared and the Fe-Au anti-bonds appeared when Au occurred in arsenopyrite by substituting As or S. Moreover, the total energy was increased when Au occurred in arsenopyrite. It resulted that Au-bearing arsenopyrite crystal was easier to be broken than before.

Keywords：simulation study; Density Function Theory; Au; occurrence state; arsenopyrite

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