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Density functional based tight binding (DFTB+) studies of pentlandites (Fe, Co, Ni)₉S₈ minerals

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Density functional based tight-binding method (DFTB+) is code which can calculate the small atoms electronic properties and molecular dynamics of large structures. We used parameterization techniques to study pentlandite minerals and large structure using a density functional based tight-binding (DFTB+) method. Pentlandite structures are the transitional-metal sulfides of the Fe, Ni group elements, and Co₉S₈being the only known binary phase. We developed sets of parameters for Co₉S₈, Fe₉S₈, Ni ₉S₈, and Fe₄Ni₅S₈mineral compounds. However Co-S, Fe-S, Ni-S and S-S interaction pairs produced a good bond lengths and the lattice parameters of these pentlandites minerals sulfides gave a good agreement of DFT-based calculations and experimental results. We calculated molecular dynamics on (1 1 1) surface Co₉S₈ nanoparticle from 300K to 1000K, and showed a zero band gap at a higher temperature. Supercell of pentlandite structure Fe₄Ni₅S₈ with 1864 atoms, the density of states (DOS) showed a band gap structure with a zero Fermi energy. We alloyed supercell of pentlandite structure Fe₄Ni₅S₈ of 1864 atoms with oxygen and changed the electronic properties with significance importance properties of pentlandites minerals.

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Level for award
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N/A

Main supervisor (name and email)
and his / her institution

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Would you like to
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no

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