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Electronic and vibrational stability of M9S8 (M= Ir, Rh,) pentlandite-like structures: ab-initio study.

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Metal sulphides are important in many fields of science such as in metallurgy, materials science, geochemistry, physics, geology and chemistry. They serve as a source of the world's precious metal-bearing minerals that are economically and industrially significant. The Bushveld Complex has the largest concentration of platinum group elements (PGEs) which are hosted in the base metal sulphides (BMS). Pentlandite minerals are known to host such precious metals, either as solid solutions or as intergrowths. The existence of the PGEs in pentlandite structure is a promising formation of new pentlandite-like system. Thus there is a need to investigate the formation and stability of Ir9S8 and Rh9S8 in pentlandite-like structures. In this study ab-initio density functional theory was used to investigate phase stabilities of Ir9S8 and Rh9S8 pentlandite-like systems. The calculated elastic constant of the systems were found to satisfy the mechanical stability of cubic systems. Furthermore, the heat of formations calculated were found to be negative, suggesting stability. The density of states of showed high stability in these systems as their Fermi energy falls into the pseudo-gap, this is in agreement with previous work. Moreover, their phonon dispersion curves appeared to have no negative frequencies (soft modes), hence they are vibrational stable. These findings provided new knowledge that establishes the stability of the PGEs existence in pentlandite-like structure that could be applicable in geological search of such phases.

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MSc

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