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First-principles study on interaction of O2 with (100) surfaces of sperrylite and platarsite minerals

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Platinum group minerals (PGMs) are usually exposed to oxidation due to weathering and aging and there is lack of understanding in their interaction with oxygen. We have employed the density functional theory (DFT) to investigate the oxidation mechanism of sperrylite (PtAs2) and platarsite (PtAsS) (100) surface. The computed surface energies and morphologies for sperrylite and platarsite models, depicted the (100) plane as the preferred cleavage. We have adsorbed the oxygen molecule at different adsorption sites to attain the most exothermic site and preferred bonding mode. The oxidation mechanisms of the (100) surfaces of sperrylite and platarsite favoured the mono atomic oxygen bonding, which resulted from the dissociation of the O2 molecule on the surfaces. The adsorption energies was more exothermic for PtAs2 (100) surface oxidation (−217.19 kJ.mol−1), compared to platarsite (−181.86 kJ.mol−1), suggesting that sperrylite highly oxidises than the platarsite mineral. These findings have demonstrated the oxidation behaviour of the sperrylite and platarsite platinum group minerals that is applicable to their weathering, and consequently how the oxidation may affect their floatability.

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Yes

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PhD

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