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Adsorption of hydroxide, water and modified collectors on sperrylite (100) surface

Organic collectors plays an important role in the recovery of platinum group minerals (PGMs) via flotation process. Sperrylite (PtAs2), is the world most common PGM and is abundant in the Platreef bushveld complex of South Africa. This mineral has been reported to be hard to float and requires detailed understanding and design of new collectors to improve its recovery. In this study we employed the Vienna Ab-initio Simulation Package (VASP) at Lengau cluster and the surface systems contained more than 120 atoms. We utilised 72 cores and the structures were converged after ten days. We investigated the interaction of hydroxide (OH-), water (H2O) and collectors at different adsorption sites on the most stable (100) surface of PtAs2. The OH- adsorption on As-top site was more exothermic (−406.31 kJ/mol), suggesting preferential adsorption on As atoms than on Pt atoms. The H2O adsorption on Pt-top site was more exothermic (−82.95 kJ/mol), suggesting that it preferred to adsorb on Pt atoms than on As atoms. The case of collectors, we have tested three modified collectors (3-thio-butyl-dithiocarbamate (3-TBDTC), butyl-carbonotrithioate (BCTT) and N-Butyl-1,3-diethylamide (NBDEA)). We observed that the adsorption of 3-TBDTC was much stronger on As-bridging (−164.63 kJ/mol). The NBDEA was found to be less exothermic with adsorption energy of −64.96 kJ/mol on As atom. The BCTT was stronger when bridging on Pt and As atoms with adsorption energy of −110.62 kJ/mol. These showed that 3-TBDTC has good collecting ability than the BCTT and NBDEA collectors. These findings pave a way for design of new collectors that can improve the recovery of hard to float PtAs2 mineral and other arsenide mineral.

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