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The adsorption of triazine collectors on sperrylite (100) surface studies by first-principles calculations

The separation of valuable minerals from the gangue minerals is still a challenge, in particular the extraction of arsenides platinum group minerals (PGMs). It has been reported that the flotation of PGMs resulted in low recovery when using traditional xanthates. This was owed to the report that the arsenides hosting the platinum group elements (PGEs) minerals are not amiable to flotation. Therefore new collectors are required to improve the recovery separation of hard to float in particular sperrylite mineral. The triazine modifications are promising reagents for mineral flotation and have not been given much attention in minerals processing. However, the adsorption of 2,6-dithio-4-butylamino-1,3,5-triazine (DTBAT), 2,6-ditrithiocarbonate-4-butylamino-1,3,5-triazine (DTTCBAT) and sodium normal butyl xanthate (SNBX) on sperrylite (100) surface were performed to identify a well performing collector molecule. This study used first-principles computational density functional theory (DFT) to determine the adsorption energies of triazine and xanthate collectors onto sperrylite (100) surface. We observed that the triazine collectors preferred to bridge on surface As and Pt atoms through the S atoms. We found that the adsorption energies were in the order: DTTCBAT (−259.29 kJ/mol) > DTBAT (−230.16 kJ/mol) > SNBX (−168.53 kJ/mol) indicating that the DTTCBAT had strong exothermic adsorption. These results showed that the ditrithiocarbamate had a great influence in the adsorption strength on the sperrylite surface. Importantly it was found that the triazine collector had strong adsorption than the xanthate, which portray a promising replacement of xanthate collector. These results paved a way for design of novel collector for sperrylite and other chalcogenide minerals to improve their recovery.

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