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Investigation of xanthate, dithiocarbamate and triazine collectors adsorptions on sperrylite and platarsite (100) surface: A DFT-D3 calculations

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The separation of valuable minerals from the gangue minerals is still a challenge, in particular the extraction of arsenides platinum group minerals (PGMs) such as sperrylite and platarsite. 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 PGMs minerals are not amiable to flotation, and therefore new collectors are required. The triazine collectors are promising reagents for mineral flotation and have not been given much attention in minerals processing. In this study, we used density functional theory with dispersion correction to perform the adsorption of sodium normal butyl xanthate (SNBX), sodium normal butyl dithiocarbamate (SNBDTC) and 2,6-dithio-4-butylamino-1,3,5-triazine (SDTBAT) on sperrylite and platarsite (100) surfaces. It was observed that the collectors preferred to bridge on surface As and Pt atoms through the S atoms on sperrylite, while on platarsite they adsorbed though mono-dentate between S atom on Pt atom. Furthermore, it was found that the adsorption energies were in the order: SDTBAT > SNBDTC > SNBX, indicating that the SDTBAT had strong exothermic adsorption on sperrylite and platarsite. Interestingly, the collectors were more exothermic on sperrylite surface than platarsite. Importantly, it was found that the triazine collector had strong adsorption than the xanthate and dithiocarbamate, which depict a promising replacement of xanthate and dithiocarbamate collectors. Therefore, these results have identified well performing collector (triazine) to improve the recovery of PGMs.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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