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Interactions of s-triazine, xanthate and dithiocarbamate collectors on platarsite (100) surface at different pH conditions: A DFT-D3 study

The study on performance of the novel 2,6-dithio-4-butylamino-1,3,5-triazine (DTBAT), normal butyl xanthate (NBX) and normal butyl dithiocarbamate (NBDTC) collector on platarsite serve as a foundation for understanding the flotation reactivity, which may be applicable in a wide range of sulphide and arsenide platinum group minerals (PGMs). This study adopted computational density functional theory (DFT) to perform the adsorption of NBX, NBDTC and DTBAT on platarsite (100) surface under neutral, alkaline and acidic conditions. It was observed that the collectors preferred monodentate adsorption mode between S atom on Pt atoms. Furthermore, it was found that the adsorption energies followed the decreasing order as: DTBAT > NBDTC > NBX, under both neutral and acidic conditions, while under alkaline conditions, the order followed as: NBX > NBDTC > DTBAT. These suggested that the DTBAT exhibited the strongest exothermic adsorption under both neutral and acidic conditions, while the NBX had strong exothermic adsorption under alkaline conditions. It was noted that the NBX collector had the strongest most exothermic adsorption energy (−413.17 kJ.mol^{−1}) which was under alkaline conditions. Therefore, these results identifies the NBX collector as a predicted well performing collector to improve the recovery of platarsite. Moreover, the alkaline conditions, is recommended for flotation recovery of platarsite mineral.

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