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EXPERIMETAL AND DENSITY FUNCTIONAL THEORY COMPARISON STUDY OF XANTHATE, DITHIOCARBAMATE AND DITHIOPHOSPHATE ADSORPTION ON SPERRYLITE SURFACE

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The comparison study on adsorption of normal butyl xanthate (PNBX), mono butyl dithiocarbamate (BDTC) and dibutyl dithiophosphate (DBDTP) on sperrylite mineral forms a basis in understanding the floatability improvement and paves a way for design of collectors that may impact a wide range of arsenide minerals. This study used a computational density functional theory (DFT) and experimental microcalorimetry approach to determine the adsorption energies of NBX, BDTC and BDTP collectors onto sperrylite mineral surface. For computational aspect, we considered the most stable surface plane of (100) surface, which had been found to give the lowest surface energy as compared to the other surface planes. We observed that the NBX, BDTC and BDTP preferred to bridge on the As and Pt atoms through the S atoms. These finding showed that the collector adsorb on the surface through both Pt and As atoms and indicated that the As atoms were significantly active in the adsorptions. The computational calculated adsorption energies were in the order: BDTC (−376.93 kJ/mol) > NBX (−369.47 kJ/mol) > BDTP (−350.97 kJ/mol), indicating that the dithiocarbamate had strong exothermic adsorption. From the microcalorimetry test we also found that the BDTC was more exothermic than the BDTP and the PNBX and the adsorption energies were in the order: BDTC (−473.50 kJ/mol) > BDTP (−392.56 kJ/mol) > NBX (−331.13 kJ/mol). These results showed that nitrogen atom in the BDTC collector had a great influence in the adsorption strength of the collector on the mineral surface. These results paved a way for design of novel collector for sperrylite and other chalcogenide minerals and suggested that nitrogen in a collector may significantly improve the affinity of the collector for better recovery.

Apply to be considered for a student ; award (Yes / No)?

Yes

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

PhD

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