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Computational study on interaction of S-allyl-N-diethyl-dithiocarbamate (ADEDTC) and s-triazine collectors on (311) surface of pentlandite (Fe5Ni4S8)

Nickel reserves are expected to run out by 2030 which contribute to various industrial applications such as stainless steel, coinage, and rechargeable batteries. Pentlandite is the primary source of nickel as well as a major carrier of platinum group elements (PGEs). The flotation of pentlandite and nickel ore has always been performed using traditional xanthates, dithiophosphate and dithiocarbamate collectors which are not so effective due to their low selectivity. Therefore, there is a need for finding a best collector that will possess both flotation power and selectivity performance. This study adopted that density functional theory (DFT) with dispersion correction by Grimme to investigate the adsorption of S-allyl-N-diethyl-dithiocarbamate (ADEDTC) and sodium dithio-butyl-amino-triazine (SDTBAT) collectors on dry Fe5Ni4S8 (311) surface. The adsorptions were performed on Ni and Fe atoms as preferred adsorptions sites. It was found that ADEDTC gave the most exothermic adsorption energy of (–460.58 kJ/mol) compared to s-triazine (–352.48 kJ/mol). Most significantly these collectors preferred to bind on Ni atoms than Fe atoms, which indicated their selectivity towards the pentlandite mineral. These suggested that ADEDTC is the best co-collector compared to s-triazine collector for utilization in the flotation of pentlandite minerals.

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