THEORETICAL STUDIES ON AIR-FROTH FLOTATION OF SULPHIDE MINERALS: INTERACTION OF DIFFERENT COLLECTORS WITH Cu^{1+}, Cu^{2+}, Zn^{2+} AND Pb^{2+} IONS

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The development of effective concentration methods of valuable minerals is important for the mining industry. The most widely used method is froth flotation. In flotation the valuable minerals are separated from the crude ore with the help of certain organic chemicals, collectors. These chemicals induce differences on mineral surfaces thus facilitating their attachment onto air bubbles. The important minerals are then collected with the froth. The process is very complicated because it occurs at the interfaces of gas, liquid and solid phases. The overall understanding of surface structures of minerals and properties of collectors in the atomic level assists in modelling the flotation mechanisms.

In this work ab initio and density functional methods have been applied to study the interaction of collectors with Cu^{1+},Cu^{2+},Zn^{2+} and Pb^{2+} ions. The collectors are ethylxanthate ($CH_3CH_2OCS_2^-$), ethyl trithiocarbonate ($CH_3CH_2SCS_2^-$), dithiobutyric acid ($CH_3CH_2CH_2CS_2^-$), ethyl dithiocarbamate ($CH_3CH_2NHCS_2^-$), diethyl dithiocarbamate ($(CH_3CH_2)_2NCS_2^-$), diethylphosphinecarbodithioic acid ($(CH_3CH_2)_2PCS_2^-$), and diethoxyphosphinecarbodithioic acid ($(CH_3CH_2O)_2PCS_2^-$). The strongest interaction with all the metal ions was found to diethyl dithiocarbamate. The results give preliminary information on the effect of the collector structure on the interaction between sulphide minerals and collectors. The results also help in tailoring suitable collector molecules for flotation.