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Computational and experimental study on heats of adsorption of MBT, MBO and MBI onto pyrite mineral surfaces

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The adsorption of heterocyclic collectors such MBT, MBO and MBI on pyrite mineral surface are paramount in order to establish understanding on the floatation reactivity that may be applicable in a wide range of sulphide minerals. This study explores the heats of adsorption of heterocyclic collectors onto pyrite mineral surfaces. The computed heat of adsorption energies of collectors indicated that the order of adsorption decrease as: MBO > MBI > MBT on both (100) and (111) surfaces. In the case of the pyrite (100) surface, the MBT adsorbed through the exocyclic sulphur atom, while MBO and MBI adsorbed through the exocyclic sulphur and N atoms onto the 5-coordinated Fe atom. The pyrite (111) surface was found to be more reactive and different adsorption mechanisms were predicted, where the MBT exocyclic sulphur atom bridged on the 5-coordinated Fe and surface 2-coordinated sulphur atoms, while the N atom adsorbed on the 5-coordinated Fe atom. In the case of MBO and MBI, dissociation of the exocyclic sulphur atom from the collector occurred with subsequent interaction with the surface 5-cordinated Fe and 2-coordinated S atoms. This resulted in the collector carbon atom adsorbing on the surface 2-coordinated S atom, while the N atom adsorbed on the 5-coordinated Fe atom. The microcalorimetry experimental heats of adsorption of MBT, MBO and MBI indicated that MBI had the strongest adsorption and the order of adsorption decrease as: MBI > MBT > MBO.

HPC content

The study on adsorption of MBT, MBO and MBI collectors on pyrite surfaces was performed using materials studio CASTEP code running at the CHPC. The calculations used 72 cores running for three to four days to complete, whiles they would take more days with less core. This signifies the impact of the HPC on this study.

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