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Effect of MBT, MBO and MBI and their derivatives on pyrite (100) surface adsorption

The adsorption heterocyclic collectors such MBT, MBO, MBI and their derivatives on pyrite mineral forms a basis in understanding the reactivity that may be applicable in a wide range of sulphide minerals. This study explored the structural and atomic charges directly related to the reactivity of MBT, MBO, MBI, n-Et-MBT, n-Et-MBO and n-Et-MBI onto pyrite (100) surface. We employed the CASTEP code at Lengau cluster at the CHPC, using 72 cores. The calculations took three to four days to complete and converge. The obtained results indicated that the S and N atoms of the collectors participate significantly in bonding on the mineral surfaces. The computed adsorption energies indicated that the substitution of ethyl (–CH2CH3) group on the 6-position of the benzene ring gives the strongest adsorption for MBT and MBO, while for MBI the 5-position was the strongest. The order of reactivity was predicted to decrease as: 6-Et-MBT > MBO > 6-Et-MBO > MBI > 5-EtMBI > MBT. This showed that the substitution of ethyl group only improves the adsorption of MBT, with no improvement for MBO and MBI. The adsorption geometry predicted that the MBT and 6-Et-MBT prefer to adsorb through the exocyclic S1 atom, while the MBO, 6-Et-MBO, MBI and 5-Et-MBI adsorb on the surface Fe atoms through the S1 and N atoms. From the atomic charges we observed that the S atoms behaved as electron donor, while the Fe atoms accepted charges. These clearly showed that the 6-Et-MBT gives the strongest and exothermic interaction.

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