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WATER ADSORPTION ON PtAs2 (111) SURFACE: A GENERAL PICTURE FROM DENSITY FUNCTIONAL THEORIES

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Most of the world's supply of platinum and palladium and associated elements comes from mines within four major layered igneous intrusions: the Bushveld Complex in South Africa, the Stillwater Complex in the USA, the Great Dyke in Zimbabwe and the Noril'sk-Talnakh Complexes in Russia. The predominant PGM in the mined area of the Platreef and Merenskyite of the Bush complex in South Africa are (Pd,Pt)(Bi,Te)2, PtTe2, PtAs2, and Pd2As, respectively. The high concentrations of these minerals make it necessary to explore opportunities to maximize the recovery these minerals by flotation. The interaction of these mineral with xanthates, whereby the mineral surface is rendered hydrophobic and gas bubbles can adhere to the surface, has been utilized for many years in practical flotation systems, but this may not be the optimal approach. Industrial mineralogical studies have found platinum group minerals, such as Sperrylite (PtAs2) to be poorly recovered during flotation. Research on the flotation behaviour of Sperrylite mineral is very limited, due to their small size (<10μm), and also the scarcity of individual grains contribute to the complexity of studying fundamental interactions. This study employs ab-initio method to investigate the effect of water molecule on the low index surfaces of PtAs2. The convergent test of slab thickness, vacuum width between slabs and surface relaxation were carried out in order to obtain meaningful results. The results of the adsorption of water molecules on the low index surfaces (100), (110) and (111) are presented and discussed and compared with the available experiment.

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