Contribution ID: **213** Type: **Poster Presentation**

Computational Modelling of Platinum Arsenide (PtAs</2>)

Tuesday, 26 June 2018 15:00 (2 hours)

Compound such as cooperate, braggite, sperrylite and platarsite are important sources of platinum (Pt) and palladium (Pd) in many of the world's largest deposits of platinum group minerals (PGM). South Africa is major producer of platinum group elements (PGE), therefore research in understanding the surface chemistry and surface reactivity of this platinum group mineral is central to major mining industrial process. Sperrylite (PtAs</2>) is an important and very rare ore of mineral of platinum, but still by far the best known compound containing platinum. Industrial mineralogical studies have found platinum group minerals, such as Sperrylite (PtAs</2>) 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. We have performed density functional theory calculations within the generalized gradient approximation (GGA) to study bulk, electronic and surface properties of PtAs</2> using CASTEP code. The theoretical calculated lattice constant and bulk modulus compare very well with the available experiment and theoretical calculations. The convergence test of slab thickness and vacuum width for low index surfaces (100), (110) and (111) were carried out and the results are discussed.

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Session Classification: Poster Session 1

Track Classification: Track G - Theoretical and Computational Physics