Contribution ID: **73** Type: **Poster Presentation**

Computational Study on Surface Reconstruction of Co9S8

The Co9S8 is an important source of cobalt. The milling of the cobalt Co9S8 mineral exposes different surface and as such there are few or one surface that dominates during the crushing. The thermodynamic stable surface is less reactive and is of importance for mineral extraction. Computational method can determine the most stable surface and the preferred cleavage either through reconstruction or perfect surface cleavage. The current study investigates the surfaces of Co9S8 and their reconstruction behaviour using density functional theory (DFT). The relaxed bulk structure was found to have a lattice parameter of a = 9.790 Å, which agrees with experimental value of a = 9.928 Å. The (100), (010), (110), (101) and (111) surface were cleaved from the relaxed bulk structure and those that possessed dipole were reconstructed. The computed surface energies for the un-reconstructed and reconstructed surface showed that the reconstruction results in lower surface energies and therefore stable surfaces. In particular the reconstructed (111) surface was the most stable surface amongst the low miller index surfaces. This was also complimented by the crystal morphology, which displayed the (111) surface as the dominant plane. The study has demonstrated that the Co9S8 mineral preferred to cleave along the (111) surface and in addition showed that the reconstruction of surface is paramount in identifying the preferred mineral cleavage.

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Yes

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Hons

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials