



Contribution ID: 372

Type: **Poster Presentation**

## Computer simulation of cobalt pentlandite

*Wednesday, 13 July 2011 17:00 (2 hours)*

Cobalt pentlandite ( $\text{Co}_9\text{S}_8$ ) is the major source of cobalt. Of the several cobalt minerals, cobalt pentlandite is the most abundant and has the widest geographical distribution. This presentation looks at the computer simulation of  $\text{Co}_9\text{S}_8$  structure using different computer simulation techniques, i.e. METADISE, VASP. These techniques have been employed to investigate the effect of molecular adsorption of water on the low-index surfaces of  $\text{Co}_9\text{S}_8$ .

**Level (Hons, MSc,   
 &nbsp; PhD, other)?**

PhD

**Consider for a student   
 &nbsp; award (Yes / No)?**

No

**Would you like to   
 submit a short paper   
 for the Conference   
 Proceedings (Yes / No)?**

No

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**Session Classification:** Poster1

**Track Classification:** Track A - Condensed Matter Physics and Material Science