



Contribution ID: 372

Type: **Poster Presentation**

Computer simulation of cobalt pentlandite

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

Cobalt pentlandite (Co_9S_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 Co_9S_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 Co_9S_8

**Level (Hons, MSc,
 PhD, other)?**

PhD

**Consider for a student
 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