Contribution ID: **171** Type: **Oral Presentation**

Structural and Electronic Properties of Fe dopped Technetium Sulphide

Thursday, 10 July 2014 14:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

In this research Density Functional Theory is used to study the effect of Fe doping on the structural and electronic properties of TcS_2 in the aP1 structure. The layered nature of the system requires the inclusion of
long range van der Waals dispersion forces to yield reasonable results, comparable to experiment. Substitutional doping of
Fe at the Tc sites. Fe doping can change the electronic structure of the system from semiconductor to metal.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

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

Yes

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Session Classification: Theoretical

Track Classification: Track G - Theoretical and Computational Physics