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Structural and Electronic Properties of Fe doped Technetium Sulphide

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Abstract content
 (Max 300 words)
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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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