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Structural and Electronic Properties of Fe dopped Technetium Sulphide

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Abstract :

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.

Award :

Yes

Level :

PhD

Supervisor :

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Paper :

Yes

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