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Computational studies of palladium/platinum sulfide using solid-solution approach

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Abstract content
   (Max 300 words)

Platinum group metals particularly palladium and platinum are used for low resistance ohmic contacts in semiconducting electron devices. It is important to understand the stabilities of the structure and its different compositions. The structural, electronic and energetic stabilities of PtS and PdS have been studied using the planewave pseudo-potential calculations, where the visual crystal approximation was invoked. The equilibrium lattice constants for both systems are in good agreement with the experimental values to within 5% agreement. The elastic constants for PtS, Pt₉₀Pd₁₀S and PdS show positive shear modulus indicating mechanical stability. Furthermore, the density of states for different compositions were calculated and found to be consistent with the stability trend. Effect of pressure on Pt₅₀Pd₅₀S and Pt₂₀Pd₈₀S was investigated and show possible transformation from tetragonal to cubic.

Apply to be
 consider for a student
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No

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

Prof P. E Ngoepe, Phuti.Ngoepe@ul.ac.za University Of Limpopo

Would you like to
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 Proceedings (Yes / No)?

No

Primary author: Ms MASENYA, Mamogo (University of Limpopo)

Presenter: Ms MASENYA, Mamogo (University of Limpopo)

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