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Computational modelling studies of structural, electronic and mechanical properties of palladium sulphide

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Abstract content
   (Max 300 words)

First-principle calculations of Pd_{50-x}Pt_xS were carried out using density functional theory within the local density approximation. The structural, electronic and mechanical properties have been studied using the planewave pseudo-potential calculations, where the virtual crystal approximation was invoked. The lattice parameters were found to be in good agreement with the experimental values, within 2 % for a and c values. The results show that an increase in platinum content stabilises the Pd_{12.5}Pt_{37.5}S₅₀ structure. Furthermore, the effect of pressure was investigated at different concentrations, and the lattice parameters were found to decrease with an increase in pressure. The elastic constants show a positive shear modulus which indicates mechanical stability.

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No

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

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No

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