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The Mechanical and Structural Properties of the Pt-Ti and Ir-Ti Alloy Systems

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<p>Ab initio density functional calculations within the generalised gradient approximation (GGA) have been carried out on a wide range of phases and stoichiometries for the platinum-titanium (Pt-Ti) and iridium-titanium (Ir-Ti) alloy systems, using the Vienna Ab Initio Simulation Package (VASP). The elastic constants and elastic moduli are calculated and the electronic structure and density of states (DOS) are considered to understand the hardness and stability properties of the alloys.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

Yes

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

Yes

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