Contribution ID: **447** Type: **Poster Presentation**

Computational Phase Stability Study of Pt Alloys and Nanoparticles

Tuesday, 8 July 2014 17:10 (1h 50m)

Abstract content
   (Max 300 words)
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Special chars

The phase stability of PtCr alloy was studied by using the plane- wave pseudopotential methods. We report the structural, electronic and dynamic stability of five different phases of PtCr alloys. The elastic constants and moduli were investigated to determine the strength of the systems. The results predict the stable structures we recommend to be used for high temperature applications in aggressive environments. Our findings form the basis of stability study of Pt nanoparticles.

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Session Classification: Poster1

Track Classification: Track A - Division for Physics of Condensed Matter and Materials