



Contribution ID: 371

Type: Poster Presentation

Ab initio studies of Platinum alloyed with Chromium for jewellery applications: energetic stabilities and structural properties

The Pt-based materials are widely used in industries, including metallurgy, medicine, jewellery, fuel cells, and hydrogen evolution reactions due to their excellent electrochemical properties. However, in its pure form, platinum (Pt) is soft, thus prone to surface scratching, a concern in jewellery applications. Hence, alloying to enhance its mechanical properties is key to improving scratch resistance. This study employs first-principles calculations to investigate the effect of alloying with high corrosion resistant chromium (Cr) on phase stability, structural and mechanical properties of Pt. Calculations are carried out on FCC (face-centered cubic) structure using density functional theory (DFT) based Quantum Espresso package.

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Session Classification: Poster Session

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