Contribution ID: **219** Type: **Poster Presentation**

Structural stability and electronic properties of bulk, monolayer and bilayer PtX ₂ (X = Se and Te)

Thursday, 11 July 2019 15:00 (2 hours)

Platinum dichalcogenides PtSe₂ and PtTe₂ crystallise in layered structures. We present density functional theory calculations of the structural, stability and electronic properties of the layered bulk, monolayer and bilayer platinum dichalcogenides PtSe₂ and PtTe₂ compounds in the CdI₂ structure, space group $P\bar{3}m1$. Our calculations revealed that these compounds are mechanically and dynamically stable. The investigation of electronic properties shows that monolayer and bilayer PtSe₂ and PtTe₂ are indirect band gap semiconductors while the bulk structures are a semi-metals. The calculated band structure shows that the band gaps decrease when the number of layers increase, which allows band gap engineering for optimal photovoltaic applications.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

PhD

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