



Contribution ID: 26

Type: **Talk**

## **Charge transport, interfacial interactions and synergistic mechanism in BiNbO<sub>4</sub>/MWO<sub>4</sub> (M = Zn and Cd) heterostructures for hydrogen production: insights from a DFT+U study**

*Monday, 4 December 2017 14:00 (20 minutes)*

### **HPC content**

All calculations were performed using the Cambridge Serial Total Energy Package (CASTEP) code[1] implemented in Materials Studio 2016 [2] with the plane-wave ultrasoft pseudopotentials method [3] and Perdew-Burke-Ernzerhof (PBE) functional for the exchange and correlation contribution [4]. A plane-wave basis set was used to describe the valence electronic states. All the simulations were done using the resources provided by the Centre for High Performance Computing (CHPC), Rosebank, Cape Town [5].

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**Session Classification:** Material Science

**Track Classification:** Materials Science & Physics