Contribution ID: **26** Type: **Talk**

Charge transport, interfacial interactions and synergistic mechanism in BiNbO4/MWO4 (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].

Primary author: Mr OPOKU, Francis (Department of Applied Chemistry, University of Johannesburg)

Co-authors: Dr VAN SITTERT, Cornie (North-West University); Dr GOVENDER, Krishna (CHPC); Prof. GOVENDER, Penny (Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa)

Presenter: Mr OPOKU, Francis (Department of Applied Chemistry, University of Johannesburg)

Session Classification: Material Science

Track Classification: Materials Science & Physics