Contribution ID: **183** Type: **Oral Presentation**

Ferromagnetism in Chromium-doped Rutile, Anatase and Brookite phases of Titanium dioxide

Tuesday, 30 June 2015 15:20 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

TiO2 doped with Cr has been investigated using density functional theory with the Hubbard term (DFT+U), In addition to electronic properties, we have also investigated the magnetic properties Cr-doped TiO2. Among the crystal structure investigated includes rutile, anatase and brookite TiO2. From the study we observed that, between 0-5% Cr doping, the systems displayed a paramagnetic behavior while between 6-8% the systems exhibit ferromagnetic characteristics. The magnetic moment was found to increase with the increase in doping percentage upto 6%, above 6% the magnetic moment remained constant (˜2μB) indicating magnetic saturation. The anatase structures highly favors Cr doping than rutile and brookite.

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

Yes

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

PhD

Main supervisor (name and email)
and his / her institution

Francis Dejene
dejenebf@qwa.uovs.ac.za
University of the Free State-Qwaqwa campus, Department of physics

Would you like to <br> submit a short paper <br> for the Conference
 Proceedings (Yes / No)?

No

Please indicate whether
this abstract may be
published online
(Yes / No)

Yes

Primary author: Ms MULWA, Winfred Mueni (University of the Free State-Qwaqwa campus, Department of physics, Private Bag x13, Phuthaditjhaba, 9866, SOUTH AFRICA)

Co-author: Dr OUMA, CECIL N.M (University of Pretoria, Department of Physics, Private Bag x20, Hatfield, Pretoria, 0028, SOUTH AFRICA.)

Presenter: Ms MULWA, Winfred Mueni (University of the Free State-Qwaqwa campus, Department of physics, Private Bag x13, Phuthaditjhaba, 9866, SOUTH AFRICA)

Session Classification: DPCMM

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