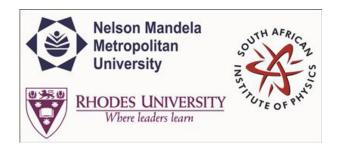
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Ferromagnetism in Chromium-doped Rutile, Anatase and Brookite phases of Titanium dioxide

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

Abstract content
 (Max 300 words)
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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 ($^{\circ}2\mu B$) indicating magnetic saturation. The anatase structures highly favors Cr doping than rutile and brookite.

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