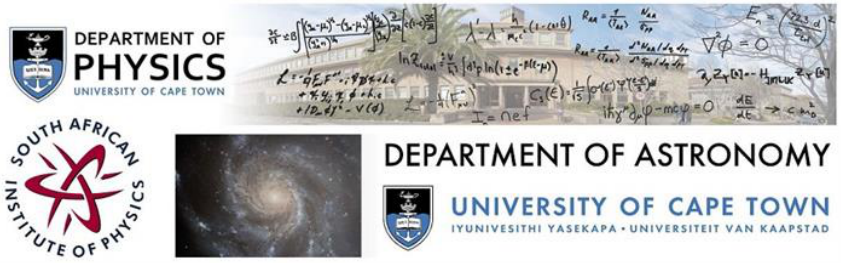

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Electronic structure and bandgap of gamma-Al2O3:Ce compound using LDA+U exchange potential

Tuesday, 5 July 2016 14:40 (20 minutes)

Abstract content
   (Max 300 words)
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Gamma-Al2O3 is a porous metal oxide and described as a defective spinel with some cationic vacancies. In this work, we calculate the electronic density of states and band structure for the bulk of this material doped with Cerium. The calculations are performed within the density functional theory (DFT) with the Hubbard correction U (DFT+U) as implemented in the quantum ESPRESSO code. The Kohn-Sham equations are solved self-consistently, employing local density approximation (LDA) with the Hubbard U correction (LDA+U) for the exchange-correlation potential. We show that LDA+U exchange potential as a local method can predict the bandgap in a better agreement with the experiment. Our electronic structure analysis indicates that the character of the valence band maximum mainly originates from the p orbitals of the oxygen electron atoms that are close to the vacancy. The charge density results show that the polarization of the oxygen electron cloud is directed towards aluminium cations, which cause Al and O atoms to be tightly connected by a strong dipole bond.
Key words: Bandgap, LDA+U exchange potential, DFT.

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