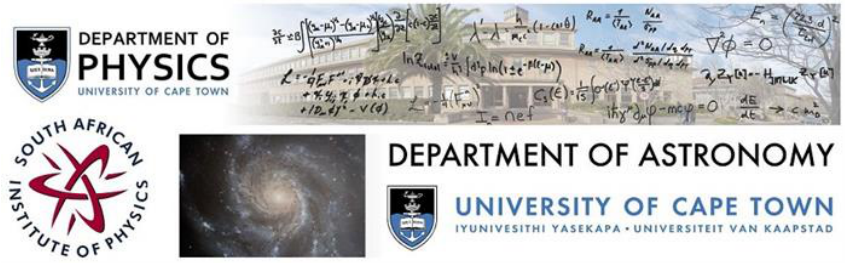

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Density Functional Theory study of stability of rutile MnO₂, VO₂ and TiO₂

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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We investigate the structural stability of metal oxides (MO) existing in similar structures, using the density functional theory (DFT) within the generalized gradient approximation (GGA). Stability (structural and electronic) properties of MO; MnO₂, VO₂ and TiO₂ tetragonal structure were determined looking at the tetragonal structure. Cell parameters of the bulk structures of the MO are in reasonable agreement with the experimental values (deviations of approximately 0.8% and -3.1% for a and c, respectively, and of 1.6 % in the cell volume). Phonon dispersion curves show that TiO₂(R), at low temperatures, is the most stable structure since it does not have vibrations in the negative frequencies.

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