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Density Functional Theory study of stability of rutile MnO_2 , VO_2 and TiO_2

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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; MnO_2 , VO_2 and TiO_2 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 TiO_2 (R), at low temperatures, is the most stable structure since it does not have vibrations in the negative frequencies.

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PhD

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

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