Ab initio Calculations of Electric Field Gradients for Transition Metal Impurities in TiO_2 *

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We present *ab initio* calculations of EFGs at impurities in a TiO_2 crystal. They are directly calculated from the self consistent charge distribution which is determined by the KKR method within the muffin-tin approximation and based on the local density approximation. Impurities in the crystal are simulated by the super-cell method. Considering the charge state of Sc, Ti, Nb, Cd, Ta impurities in the TiO_2, the experimental values were well reproduced. The electronic structure of these impurities is discussed by analyzing the calculated density of states.

Key words: TiO_2, Electric Field Gradient, Transition Metal Impurity, Band-Structure, Charge State.

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