ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ

Τίτλος

«First-principle simulations for photocatalytic nanomaterials»

«Προσομοιώσεις πρώτων αρχών για φωτοκαταλυτικά νανοϋλικά»

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Πανεπιστήμιο Κρήτης

ABSTRACT

We investigate the structure and properties of photocatalytic nanomaterials performing ab initio calculations using Density-Functional Theory (DFT). We focus on nanostructures of ZnO with substitutional Mn doping of the outmost surface layers.

We begin by extensive preparatory benchmark calculations of the atomic and electronic structure of Zn, Ti, O_2, wurtzite ZnO and anatase TiO_2 in order to find the optimum computational parameters for our simulation. We simulate O- and metal-terminated slabs of ZnO(0001) and ZnO($000\bar{1}$) surfaces with five different concentrations of Mn on the surface Zn layer. For each case, we calculate the surface energy (γ), which is a measure of the stability and the workfunction (φ), which is a descriptor of the photocatalytic activity.

We find that O-terminated surfaces are by far more stable than metal-terminated ones in all cases, and they always have higher work functions. Doping by Mn increases the stability while at

the same time it lowers the workfunction. Therefore, Mn is the ideal dopant for this system and it can be used to fine-tune the photocatalytic activity of ZnO.