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ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΟΣ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ

Τίτλος

«First-principles calculations for alloyed nanostructures»

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ABSTRACT

ZnO is one of the most popular materials for light-matter interaction applications, including photocatalysis. One of the main advantages of ZnO for such applications is that it possesses a wide band gap which is direct, located at the Γ point of the Brillouin zone. Surface alloying allows for tailoring carrier concentration at the surface level by modifying adsorption energies and activation energies for catalysis while preserving the superb electronic structure of the bulk material. Even further, surface alloying can alter the workfunction of the material and allow for it to be tuned for specific photocatalytic applications. First-principles electronic structure calculations are presented for Mn-doped ZnO with various alloying concentrations at the out-most (surface) layer of Zn atoms, while the interior of the material is kept at the ideal wurtzite structure. For each system, the surface energy and surface workfunction are calculated and trends in surface stability and surface electronic structure of this material, as well as its applications in photocatalysis are discussed. It is shown that for specific terminations of the slab, the workfunction can be tuned without significant loss in material stability.