ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ & ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

UNIVERSITY OF CRETE
DEPARTMENT OF MATERIALS SCIENCE & TECHNOLOGY

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ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ

Τίτλος

«Ηλεκτρονικές και οπτικές ιδιότητες των ZnX (X: S, Se, Te) και $Mn_xZn_yNi_zO_4$. Μια διερεύνηση από πρώτες αρχές»

«Electronic and optical properties of ZnX (X: S, Se, Te) and $Mn_xZn_yNi_zO_4$: A first principles investigation»

του Εμμανουήλ Περβολαράκη μεταπτυχιακού φοιτητή του

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπων καθηγητής κ. Ιωάννης Ρεμεδιάκης

Τρίτη 16/06/2020

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Η παρουσίαση θα διεξαχθεί με τηλεδιάσκεψη στον παραπάνω σύνδεσμο, σύμφωνα με α) την παρ. 1 του άρθρ.12 της από 11.3.2020 Πράξης Νομοθετικού Περιεχομένου (Α'55), και τις οδηγίες εφαρμογής Α Δ1α/Γποικ.28237/5.5.2020 Κ.Υ.Α (Β'1699), ΑΔΑ: ΨΠ7046ΜΤΛΗ-43Φ.

Περίληψη:

Zinc is a common material that is often used in modern materials due to its abundance, low price, non-toxicity, material stability and its great ability to alloy with most metallic elements. Zinc-containing oxides and chalcogenides are used extensively in a variety of applications. In this thesis, we consider two characteristic families of Zn-based materials: Zn chalcogenides and Zn-doped Mn_2NiO_4.

The Zn-chalcogenide family of materials (ZnS, ZnSe, ZnTe) are direct gap II-VI semiconductors which are excellent base materials for optical device technology due to their large gap and optical properties. Mn_2NiO_4, on the other hand, is a well-known material as a temperature sensor thanks to its negative temperature coefficient of resistance (NCTR) but its alloys with Zn require further investigation. In this thesis, we employ density functional theory (DFT) in the Projector-Augmented Wave (PAW) implementation to calculate the electronic structure and characteristic properties of these materials.

In the first part of the thesis we probe the structural, electronic and optical properties of the Zn chalcogenide family of materials using first principles calculations. Even though DFT can produce really accurate results for the ground state, it falls short when it comes to excited state properties like the semiconductor band-gap and the absorption spectrum. For a more accurate description, we solve the Bethe-Salpeter Equation in the GW approximation in order to include many-body effects in our calculations that arise from the electron-hole interactions like excitons.

The second part of this thesis revolves around Mn_2NiO_4 and its alloying by the Zn substitution of Mn. We calculate the ground state structure, magnetization and density of states of these materials for various concentrations Zn. We then proceed to calculate the properties of two similar material series of the $Mn_xZn_yNi_zO_4$ type. Although these alloys have very promising electronic properties, detailed simulations as well as experiments are missing. In close collaboration with experimental colleagues, we will unravel the potential of these materials for sensing applications.