**ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ**
**ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ**

**ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ**

# Τίτλος

«First-principle simulations for transition-metal dichalcogenide alloys»

«Προσομοιώσεις πρώτων αρχών για κράματα διχαλκογενιδίων μεταβατικών μετάλλων»

**Μινωτάκης Μιχαήλ**

Μεταπτυχιακός Φοιτητής

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

**Επιβλέπων καθηγητής κ. Ιωάννης Ρεμεδιάκης**

**Παρασκευή 15/03/2019**

**12:00**

**Αίθουσα τηλεεκπαίδευσης Ε130**
**Κτήριο Τμήματος Μαθηματικών και Εφαρμοσμένων Μαθηματικών,**
**Πανεπιστήμιο Κρήτης**

ABSTRACT

During the last decade, researchers have focused on two-dimensional layers of Transition Metal Dichalcogenides, MX2 where M is group IV transition metal and X is a chalcogen (S, Se, Te). Recently, it has been established that all materials in this family are semiconductors with metallic edges. An open question is how to modify these materials so that their properties, such as their band gap, satisfy the corresponding applications. The main methods that have been employed to this end are nanostructuring, strain and alloying.

In this thesis, we study alloying in 2D and 1D nanostructures. We developed a method that produces not only reliable results but also is computationally efficient. Our methodology is based on Density Functional Theory for the electronic structure and the Virtual Crystal Approximation for creating model alloys. We studied how the electronic properties and structural parameters of the 2D materials depend on the concentration of the alloying material. We have confirmed our results through test calculations with more accurate models.

We employ this method to simulate the effect of alloying on the properties of nanoribbons and study how the metallic states depend on the composition of the nanoribbon. Also, we find significant Fermi level pinning of the metallic edge compared to the interior. Furthermore, we studied how the edge energy changes with composition. Last but not least, we compared the properties of segregated versus random alloys.