ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ

Τίτλος

«Θεωρητική μελέτη και σύγκριση δομών χαμηλών διαστάσεων από διχαλκογενίδια μεταβατικών μετάλλων»

Δαβέλου Δάφνης

Μεταπτυχιακή Φοιτήτρια

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπων Καθηγητής κ. Ι. Ρεμεδιάκης

Παρασκευή, 6η Νοεμβρίου 2015,

ώρα 10:00

Αίθουσα Α210, Κτίριο Μαθηματικών και Εφαρμοσμένων Μαθηματικών,

Πανεπιστήμιο Κρήτης

Abstract

Graphene is by far the most famous two – dimensional material, that combines high electron mobility and high strength with low weight, and can be used in a variety of complex processes, such as electronics. However, the semi-metallic character of graphene and the lack of band gap may limit its applications in functional devices. Recently, more qualified candidates have emerged such as the transition metal dichalcogenides (TMDs) of the type MX_2, where M is a metal and X is chalcogen. Such materials include MoS_2, $MoSe_2$, WS_2 and WSe_2 which are also semiconductors at the 2D structure. However, previous papers on MoS_2 have shown a presence of metallic character around the edges of 1D structures.

Although the presence of metallic edge states in TMDs is well-established, it is not yet clear if these states are present in every edge or if they exist only in particular orientation of edges and/or particular reconstruction of the edges. For example, the zig-zag Mo edge seems to be the most stable one for MoS_2, and it is clear from both experiments and simulations that edge Mo atoms always shielded by S atoms. Here, we study such chalcogen-protected metal edges and find that they all possess metallic states regardless of the type of material and edge stoichiometry.

In this research, we present theoretical calculations on transition metal dichalcogenide nanostructures. We study the electronic properties and we perform first- principles calculations for the total energy, the electron density of states, the bandstructures and the wavefuctions of these materials in the 2D plane and the 1D nanoribbon configurations. For each material, we reconstruct the upper edge by adding various numbers of extra atoms and we present a comparison of all properties between the 1D and 2D materials and as a function of the adatoms number. We confirm the semiconducting character of the 2D materials and for the 1D nanoribbons we expect that all other structures will have metallic edges similarly to the case of MoS_2.