ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ & ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

UNIVERSITY OF CRETE
DEPARTMENT OF MATERIALS SCIENCE & TECHNOLOGY

**Πρόσκληση σε Δημόσια Παρουσίαση της Διδακτορικής Διατριβής της**

**κ. Δάφνης Δαβέλου**

(Σύμφωνα με το άρθρο 41 του Ν. 4485/2017)

Τη **Πέμπτη 25 Ιουλίου 2019** και ώρα **13:30** στην **αίθουσα Α210** στο κτήριο **Τμήματος Μαθηματικών και Εφαρμοσμένων Μαθηματικών**, Πανεπιστημίου Κρήτης, θα γίνει η δημόσια παρουσίαση και υποστήριξη της Διδακτορικής Διατριβής της υποψήφιας διδάκτορος του Τμήματος Επιστήμης και Τεχνολογίας Υλικών κ. Δάφνης Δαβέλου με θέμα:

## «Θεωρητική Μελέτη Διχαλκογενιδίων Μεταβατικών Μετάλλων σε Χαμηλές Διαστάσεις»

## «Theoretical Study of Transition Metal Dichalcogenides at Low Dimensions»

**Abstract:**

The isolation of graphene and other materials of atomic width caused intense interest in two – dimensional (2D) crystals. In the family of 2D materials, which is continuously growing, special place is held by the transition metal dichalcogenides MX2 where M=Mo or W and X= S, Se, Te, materials that are widely used in catalysis or as lubricants. Transition metal dichalcogenides, have been extensively studied due to the fact that they form a huge variety of structures, such as fullerenes, nanotubes, nanoribbons etc, while at the same time they present a huge field of applications from opto–electronics (for example in photovoltaics) to complex chemical reactions, such as water splitting, and biomedical applications such as drug delivery.

In this PhD thesis we study the electronic properties of quasi one – dimensional nanostructures of TMDs. We begin by studying model S structures in the tigh – binding approximation, in order to obtain insight into the electronic structure of S compounds. With Density Functional Theory as implemented by the open – source grid based projector augmented wave method (GPAW), we perform ab – initio calculations for the stability and electronic properties such as the edge energy, the density of states and the bandstructure. We find that MoS2, MoSe2, WS2 and WSe2 nanoribbons present metallic states localized

at the edges, which present a 2D band gap crossing, similar to topological insulators. From the wavefunctions at the edge we examine the physics of the metallic states according to Shockley theory and we find that the broken periodicity due to the edge formation is responsible for the electron localization. Finally, with the introduction of defects such as oxygen atoms and hydroxyl radicals in our structures, we study a more realistic behavior of our materials when they interact with atmosphere and we find that the electronic properties of 1D TMDs are robust against environmental conditions, as opposed to the 2D semiconducting energy gap which undergoes a red shift.