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

**ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΟΣ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ**

# Τίτλος

# «Theoretical Study of $MoS_2$ Defects and Dopants for Hydrogen Evolution Reaction»

της Μαρίας Μινωτάκη, μεταπτυχιακής φοιτήτριας του

Τμήματος Επιστήμης και Τεχνολογίας Υλικών του Πανεπιστημίου Κρήτης

**Επιβλέπων καθηγητής: Γεώργιος Κοπιδάκης**

## Τρίτη 08/09/2020

## 13:00

## https://teleconf.materials.uoc.gr/b/gio-dty-qwy

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.

**ABSTRACT**

Hydrogen is one of the predominant clean and renewable alternatives to fossil fuels. Efficient and sustainable hydrogen production is key to its widespread use as an energy carrier in the near future. Catalysts based on precious metals are currently used in hydrogen evolution reaction (HER). Molybdenum disulfide ($MoS_2$) is an earth-abundant, low cost, layered material with a variety of interesting properties, which depend on its dimensionality and structure. Previous work has established that while basal planes of $MoS_2$ nanostructures are inert, their edges are catalytically active in HER. In an effort to increase the number of active sites for HER in $MoS_2$ nanoparticles, Density Functional Theory (DFT) calculations were performed to examine the hydrogen adsorption ability of $MoS_2$ basal plane when modified by defects and dopants. The hydrogen adsorption free energy ($\Delta G_H$) was employed as the main activity descriptor. Introduction of a sulfur vacancy in combination with a nearby Mo-atom substitution by a transition metal enhance basal plane activity. Parameters such as hydrogen adsorption sites, hydrogen coverage, hydrogen molecule desorption mechanisms, and stability, are examined. Our findings suggest that the combination of a single Ni atom dopant and a sulfur vacancy formation in the $MoS_2$ basal plane has the maximum performance compared to several other metal dopants. Results with other transition metals provide insight into the activation mechanism of the $MoS_2$ basal plane. A volcano

relationship exists between activity descriptor and exchange current density. The relationship between activity and stability descriptors for these systems is also examined. Finally, guidelines for the design of efficient and stable $MoS_2$-based catalysts for HER using DFT calculations are outlined.