ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ & ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

UNIVERSITY OF CRETE

DEPARTMENT OF MATERIALS SCIENCE & TECHNOLOGY

ΠΡΟΣ
1) Όλα τα μέλη ΔΕΠ του Τμήματος Επιστήμης και Τεχνολογίας Υλικών
2) Τους εκπροσώπους των Μεταπτυχιακών φοιτητών του Τ.Ε.ΤΥ
3) Την Επταμελή Εξεταστική Επιτροπή
4) Όλα τα μέλη της Πανεπιστημιακής Κοινότητας

Πρόσκληση σε Δημόσια Παρουσίαση της Διδακτορικής Διατριβής της

κ. Μανιαδάκη Αριστέας

(Σύμφωνα με το άρθρο 12 του Ν. 2083/92)

Την Παρασκευή 30 Οκτωβρίου 2015 και ώρα 11:00

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θα γίνει η δημόσια παρουσίαση και υποστήριξη της Διδακτορικής Διατριβής της υποψήφιας διδάκτορα του Τμήματος Επιστήμης και Τεχνολογίας Υλικών

κ. Μανιαδάκη Αριστέας με θέμα:

«Υδρογόνο σε Νανοδομημένα Υλικά με Βάση τον Άνθρακα – Θεωρητική και Υπολογιστική Μελέτη»

«Hydrogen In Carbon-Based Nanostructured Materials – A Theoretical and Computational Study»

ABSTRACT

Carbon-based nanostructured materials (CNMs) exhibit fundamental interest and are promising candidates for numerous applications in hydrogen production, storage, and use in clean energy applications. Extensive research on carbon nanotubes, fullerenes and graphene has dramatically improved our knowledge about these materials. However, a wealth of other CNMs provide opportunities for technological advances while also presenting scientific challenges. There is strong evidence that complex nanostructures, nanoporous and disordered carbon phases, with or without other chemical substitutions, adsorb hydrogen more efficiently. Difficulties in controlling synthesis conditions, in characterization, and the complexity of these materials make their detailed theoretical study imperative.

Among these CNMs, the mixed phase of amorphous carbon (a-C) and diamond nanocrystals (n-D) has been less studied and characterized, with many of its properties remaining unexplored. We perform atomistic simulations with empirical potentials in order to create several a-C–n-D samples with different n-D sizes and a-C densities, and

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samples of ultra-nanocrystalline diamond (UNCD) with various grain sizes. We analyze the structure, stability, and mechanical properties of these nanocomposite materials and our results compare well with experiment and previous simulations. Furthermore, we study their dynamical properties to find that some pronounced features of their vibrational spectra may be observed in experiments. Finally, the effects of hydrogen in the structural and mechanical properties of these materials are investigated.

We also investigate CNMs for the adsorption and desorption of hydrogen. Recent studies have shown that transition metal dichalcogenides (TMDs) MX_2 (M = Mo, W; X = S, Se, Te) are rising candidates in the replacement of Pt as catalysts in the water splitting process. We focus on the hydrogen evolution reaction (HER) part of this process and on how Hydrogen (H) interacts with the TMDs. Specifically, we perform Density Functional Theory (DFT) calculations for MoS_2 as free standing nanostructures or positioned on a graphene substrate. These MoS_2 nanostructures as well as MoS_2/Graphene hybrid systems are investigated for their stability. Our calculations of the adsorption of H on the MoS_2/Graphene hybrid systems indicate that the effect of graphene in the adsorption process of H on MoS_2 nanostructures is quite significant.

Strain in the hybrid MoS_2/Graphene systems, inherent due to lattice mismatch, plays an important role in their properties. This leads into a theoretical investigation of the structural, electronic and dielectric properties of single-layer TMDs under various types of strain. We find that electronic band gaps decrease while dielectric constants increase for heavier chalcogens. The direct gaps of equilibrium structures often become indirect under certain types of strain. The effects of strain and of broken symmetry on the band structure are discussed. The DFT results concerning the effect of strain in the dielectric properties are theoretically explained using only structural parameters and equilibrium dielectric constant.