



**ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ**

**Τίτλος**

**« Προσομοιώσεις Μοριακής Δυναμικής Νανοσύνθετων  
Πολυμερικών Υλικών »**

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Επιβλέπων Καθηγητής κ. Ι. Ρεμεδιάκης

**Παρασκευή, 19/06/2015,**

**13:30 π.μ.,**

**Αίθουσα Α210,**

**Κτίριο Μαθηματικών και Εφαρμοσμένων Μαθηματικών,**

**Πανεπιστήμιο Κρήτης**

Abstract

The study of Polymeric Complex Materials is an intense research area due to the broad spectrum of systems, applications, length and time scales. For example, concerning hybrid Polymer/Solid systems, nanoparticles are used to modify/enhance the thermodynamics, the mechanical properties and the dynamical/rheological behavior of the entire system.

The aim of this work is to study the effect of gold, nanoparticles (NP) on polymer properties through detailed atomistic Molecular Dynamics, MD, simulations. In more detail, the structural, conformational and dynamical properties of polyethylene, PE, chains around an Au NP and a functionalized (Core/Shell) Au NP are investigated and compared to the behavior of bulk PE. Data concerning polymer density profiles, bond order parameter, segmental and terminal dynamics are reported. All polymer chain properties are examined as a function of distance from the Au NP. We find that the effect of the interface on density profile and conformational properties is from around 1.0 to 2.5 nm, whereas on local and global dynamics of polymer chains vary from around 2.0 to 4.0 nm.