ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΟΣ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ

Τίτλος

«Προσομοιώσεις πολλαπλής κλίμακας για μεταλλικά νανοσωματίδια»

«Multi-scale simulations for metal nanoparticles»

της Αγγελικής Μπουμπάκη μεταπτυχιακής φοιτήτριας του

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπων καθηγητής κ. Ιωάννης Ρεμεδιάκης

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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.

Περίληψη:

Gold is a well-known precious metal that has been used in jewelry and coins since ancient times. Being the noblest of all metals, it is resistant to oxidation and corrosion. Gold nanoparticles show several interesting properties, such as having different color depending on their size and shape and good activity as chemical reaction catalysts. Both their size and shape have key role in the efficiency of Au as catalysts.

The present master thesis presents a theoretical study of the relationship between structure and properties for gold nanoparticles. Using several different interatomic potentials and a continuum model, we calculate the surface energies of (111), (100) and (110) surfaces in good agreement to other theoretical calculations found in the literature.

We construct models of nanoparticles of high symmetry and more specifically cubic, octahedral and rhombic dodecahedral nanoparticles in several sizes, in order to understand the role of the nanoparticle' s geometry on its properties. We calculate energies that determine the shape of these nanoparticles and provide for the first time calculations for edge and vertex energies of gold nanoparticles using a new atomistic model we developed.