ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ

Τίτλος

«Μελέτη κβαντικών καταστάσεων ενός ηλεκτρονίου σε νανοδομές χρυσού»

«Single-electron quantum states in gold nanostructures»

Ραπτάκης Αντώνιος

Μεταπτυχιακός Φοιτητής

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπων καθηγητής κ. Ι. Ρεμεδιάκης

Πέμπτη, 03/11/2016,

10:00 π.μ.,
Αίθουσα Β2,
Κτίριο Χημείας,

Πανεπιστήμιο Κρήτης

Abstract

We study surface-localized electronic states (Shockley surface states) for Au and Cu. We focus on characteristic properties of these states, including their spatial distribution, their energy and their relationship to the bulk electronic states. The calculations were performed using Density Functional Theory (DFT).

We construct slabs with different number of atomic layers. These layers are parallel to the

(100) and (111) plane of FCC structure. We solved the N-electron Schrodinger equation as

implemented in the open-source package Grid-based Projector Augmented Wave method (GPAW).

We locate surface states by observing Bloch States, ($\vec{n}k$), where the probability of finding

electrons at surface atoms is much higher than the probability of finding in bulk atoms. We modify slab thickness (number of layers) and observe when the probability starts to converge.

We confirm the surface states by applying three methods. In the first method, we find the diagram of the probability density per atom. The next method was a graphical way to proove the surface state, in which we examine wavefunction plots for this method, we used VMD and

ASE. In the last method, we plot the probability density in real space. All three methods are used to confirm that particular Bloch state is indeed a surface state.

As a further validation of our method, we repeated the same process for relaxed surfaces, in which the first and the last atom of slabs are allowed to relax. We also tried a different metal (Cu), with similar results. In all cases, the simulations show remarkable agreemement with the continuous model of Shockley, although the later was designed for semiconductor surfaces.

Finally, we used the Shockley equations to determine the metal workfunction for different thicknesses of slabs. We fitted the square of the absolute value of wavefunction and applying Schockley's Surface State theory, we found values for the metal's workfunction in very good agreement to direct simulation.

This promising application of a semiconductor theory to metal nanostructures renders it a very powerful tool for analyzing and predicting quantum effects in modern nanocomposite materials.