ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ
ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

ΠΑΡΟΥΣΙΑΣΗ ΜΕΤΑΠΤΥΧΙΑΚΟΥ ΔΙΠΛΩΜΑΤΟΣ ΕΙΔΙΚΕΥΣΗΣ

Τίτλος

«Theoretical investigation of tungsten disulfide - graphene heterostructures»

«Θεωρητική μελέτη ετεροδομών διθειούχου βολφραμίου - γραφενίου»

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Επιβλέπων καθηγητής κ. Γ. Κοπιδάκης

Δευτέρα, 30/10/2017,

10:30 π.μ.,

Αίθουσα Β2,
Κτίριο Τμήματος Χημείας,
Πανεπιστήμιο Κρήτης

Περίληψη

Research in two-dimensional (2D) materials and van der Waals heterostructures gains enormous popularity across various scientific and engineering disciplines. Electrons in these materials can move in two dimensions but are confined in the out of plane direction, leading to some fascinating optoelectronic properties. In this direction of research, we present Density Functional Theory (DFT) results for the atomic and electronic structure of WS_2 monolayer, graphene and WS_2/graphene heterobilayer. We performed DFT calculations to investigate interlayer interactions and the effect of lattice mismatch in WS_2/graphene van der Waals heterostructures. We found that strain affects their binding energy and electronic structure. Examining stability and band alignment in these heterostructures with DFT is quite challenging. By using different WS_2/graphene supercells with different lattice mismatch and by unfolding their electronic band structure, we find that strain induces significant electronic properties modifications in the WS_2 layer, such as direct to indirect band gap transitions. Furthermore, in an effort to interpret recent experiments, we studied exciton effects in WS_2 monolayer using theoretical methods based on the Bethe-Salpeter equation (BSE) for 2D materials. Our excitonic spectra are in good agreement with experimental data and are affected by strain in a way which is consistent with confinement effects. Theoretical understanding of the optoelectronic properties of WS_2/graphene heterostructures complements experimental works and provides a powerful tool for exploring potential applications and devices.