Ηράκλειο 21/02/2022

Η ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΙΚΗΣ ΕΡΓΑΣΙΑΣ

της φοιτήτριας **Φωτεινής Δραγοσλή,** θα γίνει τη

<u>Πέμπτη 24/02/2022</u> και ώρα **13:00**

στην αίθουσα Β2 του Κτιρίου Χημείας

Θέμα Διπλωματικής:

« *Band-structure calculations for halide perovskites»*

«Υπολογισμοί Δομής Ενεργειακών Ζωνών για περοβσκίτες αλογόνου»

Για την παρακολούθηση της παρουσίασης δια ζώσης, το κοινό θα πρέπει να έχει τα απαραίτητα δικαιολογητικά (πιστοποιητικό εμβολιασμού, νόσησης ή rapid test).

Περίληψη:

Perovskites are a class of materials that have recently sparked a great amount of interest due to their diverse physical properties. Although there are several types of perovskites, halide perovskites have received the most attention since they can be utilized in solar cells due to their semiconductor-like characteristics. The general formula for halide perovskites is AMX3, where A is a monovalent, non-coordinating cation (Cs, CH_3NH_3 or $HC(NH_2)_2$), M is a bivalent p-block metal (Pb, Sn, and Ge are the most common) and X is a metal-coordinated halide anion.

In this work, we studied three Pb-less and inorganic perovskites ($CsSnBr_3$, $CsSnCl_3$ and $CsSnI_3$), as well as one perovskite containing Pb and an organic unit ($MAPbBr_3$) where MA is methylammonium (CH_3NH_3). We performed calculations on the band-structures of all four perovskites using Density-Funtional Theory (DFT). We focused on changes in the band- structures, particularly the bandgaps of the perovskites, as a result of changes in simulation parameters such as the lattice constants, the cut-off energy, the position of the atoms, and the spin orbit coupling. In agreement with literature, we find that, for the $CsSnBr_3$, $CsSnCl_3$ and $CsSnI_3$ perovskites, increasing the lattice constant causes an increase in the gap. In the case of the $MAPbBr_3$ perovskite, we observed that the d orbitals of Pb have no effect on the bandgap value and when the spin orbit coupling was taken into consideration, a smaller bandgap was discovered.