

Ηράκλειο 21/02/2022

Η ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΙΚΗΣ ΕΡΓΑΣΙΑΣ

Του φοιτητή **Αλαελντίν Μιχαηλίδη Μπαρακάτ**, θα γίνει τη

Πέμπτη 24/02/2022 και ώρα **14:00**

στην Β2 του Κτηρίου Χημείας

Θέμα Διπλωματικής:

«Band gap prediction & data analysis of inorganic perovskites using machine learning»

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

Abstract:

Machine learning is a very prominent approach towards material discovery based on data mining and big data analysis that has been proven extremely successful in many research fields from medicine to artificial intelligence. In the field of solid-state chemistry, machine learning can provide us with a robust method of analyzing our experimental results and making predictions on the properties and synthesis of new materials. One such class of materials is perovskites, an innovative class of semiconductor materials, which has spiked the interest of the scientific community for many years. In this project, we utilize machine learning towards the discovery of new materials combining a computational approach to identify the materials and a synthetic materials chemistry approach to attempt to verify the computational results. We focus on the study of inorganic perovskites seeking to discover new compounds with desirable optoelectronic properties in the visible spectrum for employment in photovoltaic research. We use machine learning as an alternative method to other computational as well as test-and-trial methods, and we find that our machine learning methodology provides a higher accuracy in the prediction of photoactive perovskites. By employing machine learning on analyzing and predicting properties of perovskites, we have successfully surpassed the effectiveness of conventional theoretical methods, such as DFT.