Ηράκλειο 20 Οκτωβρίου 2022

ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΙΚΗΣ ΕΡΓΑΣΙΑΣ

Της φοιτήτριας Sophia Thiele, θα γίνει την

Τρίτη 25/10/2022 και ώρα **12:00**

στην αίθουσα Συνεδριάσεων του Τμήματος Επιστήμης και Τεχνολογίας Υλικών στο κτήριο Τμήματος Μαθηματικών και Εφαρμοσμένων Μαθηματικών

Επιβλέπων: Γεώργιος Κοπιδάκης

Θέμα Διπλωματικής:

«Modeling Carbon Nanostructures with Empirical Interatomic Potentials»

Περίληψη:

Carbon based materials and nanostructures are an important part of scientific research. Carbon is ubiquitous in nature, from the living organisms, which are all based on organic compounds, to the universe, where it is the fourth most abundant element. Its atoms have the ability to form diverse bonds resulting in various allotropes which also play a crucial role in materials science and engineering. Understanding and simulating several different bonding environments is a challenge for theory and computation and considerable effort focused on developing reliable and transferrable interatomic potentials for classical molecular dynamics (MD) simulations. This thesis pertains to the application of classical MD using such empirical potentials to create materials and molecules consisting of carbon and hydrogen, determine their basic structural and dynamical properties, and compare the results with other theoretical methods, such as density functional theory and tight-binding, as well as experiment. More specifically, structure, bond lengths and vibrational spectra for diamond, graphene and its nanoribbons, methane, benzene and hydrocarbon chains were examined with MD simulations using bond order interatomic potentials. The simulation package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) was used for the MD and in-house software was developed for the calculation of vibrational spectra from the results of MD simulations using Fast Fourier Transform. Systematic comparison of results shows overall agreement between empirical potentials and experiment, with very few exceptions, where more accurate first principles methods should be used. Moreover, vibrational spectra are analyzed in terms of temperature, normal modes, and localized excitations.