SYLLABUS
"SIMULATIONS BY THE METHOD
OF *AB INITIO* MOLECULAR DYNAMICS"

National Academy of Sciences of Ukraine

Institute for Condensed Matter Physics

Speciality: 104 Physics and astronomy

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Course Description

The course presents methods of computer simulations within the density functional theory and is divided into two parts. In the first part, a detailed study of the density functional approach and algorithms for calculating electronic spectra within the framework of this formalism is presented. An important section here is a detailed study of electron-ion effective interactions (pseudopotentials) and methods of their generation. Pseudopotentials as input interactions are the basis for further understanding of the method of *ab initio* molecular dynamics, which is considered in the second part of the course. PhD students will have the opportunity to get acquainted with the most popular modern methods of basic modeling based on the Car-Parrinello methodology and the method of direct minimization of electronic degrees of freedom. Practical skills in working with software packages for *ab initio* simulations should consolidate the theoretical material.

Course Goals

The goal of this course is to master the theoretical and practical bases of the method of *ab initio* simulations for solids and disordered systems. The practical application of methods within the electronic density functional approach will allow modeling atomic-scale dynamics on single- and multiprocessor computers, which is necessary to explain processes in nanophysics and many other important areas of modern science, such as chemistry, biophysics, geophysics. The practical applications of the methods of pseudopotentials and ab initio computer simulations will allow modeling the processes of chemical bond formation, the formation of equilibrium structures from the first principles, calculations of electronic transport and polarization in disordered systems.

As a result of studying the course, the PhD student must be able to demonstrate the following learning outcomes:

Know the fundamental differences and limits of application of quantum Monte Carlo methods and *ab initio* molecular dynamics;

Know the basic algorithms of *ab initio* simulations;

Know the basic conceptual approaches to the applicability of the electron density functional and the applicability of this approach in computer modeling from the first principles;

Be able to develop computer codes for calculating the electronic properties of systems in different aggregate states.

Structure of the course

Components of the course	Total hours
Number of credits/hours	3/90
Hours of classes, including:	48
• lectures, hrs.	16
• seminars, hrs.	16
• calculus, hrs.	-
• laboratory simulations, hrs.	16
Hours of self-work, including:	42
• control tests, hrs.	-
• calculus, hrs.	-
• individual scientific study, hrs.	18
• preparation to lectures, laboratory simulations and control tests, hrs.	24
Exam	1
Modules	-

Part of class work in percents – 53.3%

Detail description of the course

Lectures

№	Title of the topics	Hours
1	**Formalism of the electron density functional** The concept of adiabaticity for electronic states. Electronic density functional theory. Kohn-Sham equation. The concept of exchange-correlation potential. Limits of applicability of the theory of electron density functional. Local and gradient approximation for the exchange-correlation functional.	4
2	**Effective electron-ion interactions for *ab initio* simulations** The concept of pseudopotential. Model and *ab initio* pseudopotentials. Norm-conserving pseudopotentials. Generation of norm-conserving pseudopotentials. Vanderbilt's ultrasoft pseudopotentials. PAW potentials. Existing libraries of pseudopotentials.	4
3.	***Ab initio* molecular dynamics** Basic principles of *ab initio* simulations. Hellman-Feynman forces. Car-Parrinello method. Fictitious dynamics of electronic degrees of freedom. Ensembles in *ab initio* molecular dynamics. Molecular dynamics by the method of energy minimization on the Born-Oppenheimer surface. Algorithms of conjugate gradients and direct minimization of electronic subsystem.	4
4.	**Calculation of properties of systems from first-principle modeling of molecular dynamics** Electron-ion distribution functions and structure factors. Optic conductivity. Thermal conductivity. Calculations of polarization for nonmetallic systems. Calculations of high-frequency contributions to the dielectric permittivity of systems.	4
Total hours		16

Calculus

№	Title of the topics	Hours
1	Construction and calculation of effective interactions for their applications in computer simulations	8
2	Microscopic models of dynamic processes in consensed matter	8
Total hours		16

Seminars

№	Title of topics	Hours
1	Choice of the algorithms for simulations of *ab initio* molecular dynamics.	4
2	Calculations and analysis of time correlation functions	4
3	Construction of norm-conserving pseudopotentials	4

4	Application of Wannier functions for analysis of chamical bonds in ab iniio molecular dynamics	4
Total hours		16

Homework

№	**Title of works**	Hours
1.	Individual scientific study (thematic presentations)	18
2.	Preparation for classes and control activities	24
Total hours		42

Explanation of grading system

Maximal grade in points						
Semester control				**Exam**		**Totally**
Lab	**Calculus and seminars**	**Homework**	**Total points**	**Written component**	**Oral component**	
-	10	10	20	-	80	100

Sample Grade Cutoffs

88% A
80% B
70% C

Textbooks

1. R. G. Parr, W. Yang. ***Density-functional theory of atoms and molecules*.** Oxford University Press, Oxford, 1989
2. D.Frenkel, B.Smit. ***Understanding Molecular Simulation.*** Academic Press. SanDiego,1996
3. R.M. Martin. ***Electronic structure. Basic theory and practical methods.*** Cambridge University Press, 2012
4. D. Marx, J. Hutter. ***Ab Initio Molecular Dynamics (Basic Theory and Advanced Methods).*** Cambridge University Press, 2009