Course Name/Kode: **ILT 533 DENSITY FUNCTIONAL THEORY I**								ADVANCED TECHNOLOGIES	
Semester	Teaching and Learning Methods							Credit	
	Theory	App.	Lab.	Project	Homework	Other	Total	Credit	ECTS Credit
1-2	42				30	76	188	**3**	**7.5**
Language	Turkish								
Compulsory/ Elective	Elective								
Prerequisites	None								
Course Content	Basic concepts of quantum mechanical calculations. The Hohenberg-Kohn Theorem. The Kohn-Sham equations. Exchange energy. Correlation energy. Kohn-Sham eigenvalues. Approximations.Local density approximations. Spin density functional theory. Time dependent density functional theory. Software tools. Theoretical calculations on the some organic molecules. Analysis of calculations.								
Course Objectives	To teach the basic principles of quantum-mechanical density functional theory which is successful and popular approaches with an application. To teach appropriate software tools for calculations of density functional theory.								
Learning outcomes and competences	To establish the relationship between theory and practice, do interdisciplinary work, gain knowledge about current issues and gain the ability to provide oral and written exercises.								
Textbook and /or References	1. D. S. Sholl, J. A. Steckel "Density Functional Theory" John Wiley & Sons (2009) 2. J. S. Foresman, E. Frisch "Exploring Chemistry with Electronic Structure Methods" Gaussian, Inc., Second Edition. 3. M. I. J. Probert "Computational Quantum Mechanins" 4. K. Capelle "A Bird's Eye View of Density-Functional Theory"								

Assessment Criteria		***If any, mark as (X)***	**Percentage (%)**
	Midterm Exams	X	30
	Quizzes		
	Homeworks	X	20
	Projects		
	Term paper	X	10
	Laboratory Work		
	Other		
	Final Exam	X	40

Prepared by	Assist. Prof. Nurgül SEFEROĞLU
Week	**Subject**
1	Basic concepts and the Schrödinger Equation
2	Functionals and derivatives
3	Hohenberg-Kohn Theorem
4	Kohn-Sham equations
5	Exchange energy
6	Correlation energy
7	Kohn-Sham eigenvalues
8	Approximations
9	Local density approximation
10	Spin density functional theory
11	Time dependent density functional theory
12	Software tools
13	Theoretical calculations on the organic molecules
14	Analysis of calculations