MODELING of NANOSTRUCTURES & MATERIALS – Summer Semester 2013

List of Lectures

1) Introduction to Computational Science, Computational Materials Science, Modeling of Nanostructures

2) Density Functional Theory – The Key to the Computational Materials Science, The Basics

3) Kohn-Sham realization of DFT, Functionals, Generelizations of K-S Equations, Examples of Calculations

4) Kohn-Sham Method with plane-waves & pseudopotentials

5) Kohn-Sham Method with plane-waves & pseudopotentials (cnt.), Introduction to Molecular Dynamics

6) Molecular Dynamics (MD), Classical vs. Ab Initio MD, Born-Oppenheimer MD, Car-Parrinello MD, Thermostats, Time evolution of Atomic Positions in MD

7) Molecular Dynamics & Coarse Graining, Tight-Binding Methods

8) Kohn-Sham equations, Concept of Muffin-Tin Potentials, LAPW and FP-LAPW Method, LMTO Method

9) Basics of the Alloy Theory, Continuum Methods in Materials Science

10) Band Gap Energies in DFT, Further Developments of DFT methods