NanoDFT'09 Program:

09 Aug, Sunday: Registration + Check in to İYTE dorms

		10 Aug, Mon	11 Aug, Tue	12 Aug, Wed	13 Aug, Thu	14 Aug, Fri	15 Aug, Sat	16 Aug, Sun
Lecture	**09:30 – 10:15**	OPENING	S.Ö.-L2	H.T.-L1	H.T.-L3	H.T.-L5		
Lecture	**10:15 – 11:00**	O.G.-L1	S.Ö.-L3	H.T.-L2	H.T.-L4	H.T.-L6	**10:00 – 12:00** **Tutorial** H.T.-E.M.	
Cof.-Tea	**11:00 – 11:15**							
Lecture	**11:15 – 12:00**	K.G.-L1	K.G.-L2	D.T.-L1	E.M.-L1	T.Ç.-L1		
Lunch	**12:00 – 14:00**							FREE (Social event?)
Lecture	**14:00 – 14:45**	S.Ö.-L1	K.G.-L3	D.T.-L2	E.M.-L2	T.Ç.-L2	**14:00 – 17:00** **Tutorial**	
Cof.-Tea	**14:45 – 15:15**							
Tutorial	**15:15 – 17:30**	K.G.-T1	K.G.-T2	H.T.-T1	H.T.-T2	T.Ç.-T1		

		17 Aug, Mon	18 Aug, Tue	19 Aug, Wed	20 Aug, Thu	21 Aug, Fri
Lecture	**09:30 – 10:15**	T.S.-L1	I.R.-L3	M.G.-L3	M.G.-L5	S.B.-L1
Lecture	**10:15 – 11:00**	T.Y.-L1	I.R.-L4	M.G.-L4	M.G.-L6	S.B.-L2
Cof.-Tea	**11:00 – 11:15**					
Lecture	**11:15 – 12:00**	I.R.-L1	M.G.-L1	T.Y.-L2	D.T.-L3	S.B.-Overview
Lunch	**12:00 – 14:00**					
Lecture	**14:00 – 14:45**	I.R.-L2	M.G.-L2	T.Y.-L3	D.T.-L4	
Cof.-Tea	**14:45 – 15:15**					DEPARTURE
Tutorial	**15:15 – 17:30**	I.R.-T1	I.R.-T2	M.G.-T1	D.T.-T1	

Lecturers, Topics:

Ini.	Name	Affiliation	Topics
D.T.	Daniele TOFFOLI	METU	Hatree-Fock and beyond: Chemical methods
E.M.	Ersen METE	Balıkesir U.	DFT in practice: plane wave expansion, pseudopotentials and basic iterative algorithms
H.T.	Hande TOFFOLI	METU	Basics of DFT and Plane wave methods
I.R.	Ivan RUNGGER	Trinity C., Ireland	Quantitative theory for electron transport in nanodevices: Smeagol code
K.G.	Kaan GÜVEN	Koç U.	Numerical Methods
M.G.	Matteo GATTI	ETSF, France	TDDFT/GW-BSE
O.G.	Oğuz GÜLSEREN	Bilkent U.	Introduction and applications of DFT
S.B.	Stefano BARONI	SISSA, Italy	Density-functional perturbation theory
S.Ö.	Serdar ÖĞÜT	UIC, USA	Real Space Methods
T.Ç.	Tahir ÇAĞIN	TAMU, USA	DFT applications on functional materials
T.S.	Tuğrul SENGER	İzmir IT	Introduction to electron transport in molecular structures
T.Y.	Taner YILDIRIM	NIST, USA	Exchange interaction on magnetic clusters: LDA+U and beyond

Location:

All lectures and tutorials will be at İYTE Physics Department.

Lectures: G-110 Seminar Room

Tutorials: G-148 Computer Lab

Tentative contents of the lectures:

Hande Toffoli

1st day, morning session: Basic concepts
1) The variational principle (if not already covered by someone else)
2) Fundamental concepts in solid state: reciprocal space, BZ, band structure, DOS
3) The functional derivative (again if not already covered)
4) The many-body Hamiltonian

1st day, afternoon session: Hands-on + exercises
1) Overview and examples in Octave/Matlab
2) An example for the variational principle solved traditionally
3) An example for the variational principle solved using numerical integration
4) Simple exercises in BZ finding, DOS and band structure

2nd day, morning session: Basics of DFT
1) The Hohenberg-Kohn theorem
2) Brief mention of extensions to the HK theorem such as the Levy construction
3) Brief mention (for now) of exchange and correlation
4) Total energy in terms of density
5) The Kohn-Sham equations
6) The concept of basis expansion

2nd day, afternoon session: Hands-on + exercises
1) Problem-solving period: Various problems related to the topics covered in the morning.

3rd day, morning session: Input structure
1) PW expansion: example basis expansion for a couple of terms in the Hamiltonian
2) The pseudopotential idea
3) Ideas behind input parameters: cutoff, BZ integration, SCF parameters such as mixing etc.
4) Some more discussion on exchange and correlation

3rd day, afternoon session: Hands-on PWSCF
1) Lattice constant of diamond
2) Band structure and DOS of graphene

Daniele Toffoli

An overview of correlated methods in quantum chemistry, somewhat beyond DFT, such as Coupled Cluster, Configuration interaction, and Moller-Plesset. An interesting topic would be response theory, but it should be already covered in TDDFT. In the modern literature of, for example, Coupled Cluster, everything is done in second quantization, so I would also like to introduce and use the tool in the lectures. I think the level is accessible to master students.

Here is the plan.

I day: Hartree-Fock Theory in first quantization
1) Slater-Condon rules
2) Derivation of the closed shell HF equations.

3) The dissociation problem and its unrestricted solution
4) Beyond HF: the standard models (brief description of CC, CI, and MP2)

II day: Introduction to second quantization
1) Second quantization
2) Orbital rotations
3) Hartree-Fock theory in second quantization
4) Basis sets

In addition there can be a session with exercises on the topic presented.

III) day: Coupled-cluster theory
1) The concept of size extensivity
2) Coupled cluster theory
3) Moller-Plesset perturbation theory

If permitted a short discussion on molecular properties and methods of calculations. Of course all the methods are then compared with DFT. In addition there can be hand-on session on popular quantum chemistry software (GAMESS, DALTON)

Matteo Gatti

TDDFT / GW+BSE
I normally deal with theoretical spectroscopy which involves the study of the excited states.
In this context, a general introduction about time-dependent DFT and approaches based on Green's functions (GW and Bethe-Salpeter equation) is always instructive.
The focus could be on the calculation of optical properties of finite systems, comparing the different approaches we can adopt, from DFT and effective-medium theories to more advanced approximations.

You can find the lectures online:
http://www.cecam.org/workshop-314.html

Serdar Öğüt
First Principles Real-Space Methods for Predicting Electronic and
Optical Properties of Confined Nanostructures

Clusters (Si, Ge, Ag, Au, etc) and nanocrystal (Si_nH_m), real-space method (PARSEC).
Time-dependent density functional theory (real-space frequency domain implementation) and GW+BSE (real-space implementation)

Ersen Mete

"DFT in practice" tutorial.
"idea of pseudopotentials, xc functionals ve basic minimization schemes"

"DFT in practice"
1. The plane wave basis set
2. Pseudopotentials
3. Iterative minimization algorithms

Taner Yıldırım

Magnetic cluster/molecular-magnets, exchange interaction. DFT+LDA+U method.

Kaan Güven

Numerical Methods.

Stefano Baroni

I could lecture 2-3 hrs on density-functional perturbation theory.

Ivan Rungger

The planned lecture is along the lines of "Non equilibrium Green's functions for electron transport in nanodevices" (or something like "Quantitative theory for electron transport in nanodevices"), and the tutorials on "Using the Smeagol code for quantitative electron transport calculations"

Tahir Çağın

DFT applications on functional materials.

Oğuz Gülseren

Introduction and applications of DFT.

Tuğrul Senger

Introduction to electron transport in molecular structures.