Introductory Training on Theoretical Spectroscopy

Summary

Electronic excitations, caused for example by irradiation with electrons, light or modern photon sources (synchrotron, ultra-fast lasers), are key quantities for the study of materials, ranging from solids to atoms, from surface to nanoscale systems.

Experimental techniques measuring electronic excitations have seen rapid progress (high spatial resolution, short measurement time, low temperature), which continuously requires and stimulates a more precise theoretical description and analysis. The joint use of theory and computer simulation has in fact, over the last decades, permitted to achieve big improvements in the description of optical and electronic properties of finite and infinite systems.

Scopes

The main scope of this introductory training day is to provide attendees with both the theoretical foundations and the knowledge about ab initio calculations. After a brief introduction about the programmes and training solutions proposed by the **European Theoretical Spectroscopy Facility** (ETSF, **http://www.etsf.eu**), theoretical approaches along two different lines will be presented: on one side, methods based on density functionals and on the other side, methods based on Green's functions in many-body perturbation theory. The emphasys is on excited states theory and calculations, in particular valence electron excitations. The aim is not to learn technical details of theoretical methods, but to get insight about the fundamental ideas, in-principle possibilities and limitations, and in-practice performance and shortcomings.

The aims of this tutorial are hence to:

- *give an overview over the ETSF training possibilties*
- *give an overview of the theoretical points of view concerning valence electron spectroscopy*
- *present the two most important approaches for electronic excitations*
- *present the computational codes involved in these calculations*
- *illustrate typical applications (presenting successes and shortcomings), as well as new frontier applications*
- *present the capabilities of the ETSF, helpful for eventual user projects.*

Program

09h30 - 09h55 Introduction to ETSF: training solutions
09h55 - 10h00 An ETSF training project: experience of an undergraduate student
10h00 - 10h10 Introduction to *ab initio* approaches for electronic structure calculations
10h10 - 10h40 Density Functional Theory: description through electron density
10h40 - 11h10 *Caffeine Break*
11h10 - 11h40 Green's Functions theory: description through (quasi)particles
11h40 - 11h50 Industry meets Theory: experience of a PhD student

Lunch

The afternoon is dedicated to the presentation of ETSF "beamlines", i.e. to theory and applications centred around particular experimental approaches.

13h30 - 14h20 Photo-emission beamline
14h20 - 14h30 Presentation of the ETSF liveCD
14h30 - 15h20 Optics beamline
15h20 - 15h50 *Caffeine break*
15h50 - 16h40 Loss Spectroscopy beamline
16h40 - Discussions

Thursday 19/11/2009
Amphi Fresnel
École Polytechnique
Palaiseau

Please confirm your venue before 05/11/2009

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