

THEORETICAL SPECTROSCOPY

The ETSF Users' Newsletter

Invitation to all ETSF Users: 14th ETSF Workshop

The 14th ETSF Workshop entitled "Ab-initio tools for the characterization of nanostructures" will take place in Evora (Portugal) on September 14-19. This annual ETSF Workshop focuses on topics related to the first-principles description of electronic excitations and spectroscopy, and it is presently regarded as the main scientific event in the field.

The next ETSF workshop will be the first opportunity to exchange ideas between ETSF scientists and users and foster future collaborative projects. Thus, the participation and scientific contributions by ETSF users are specially welcome this year. Furthermore, a round-table meeting between users and ETSF representatives will take place during the Workshop. This round-table will serve to discuss and collect suggestions with the aim of improving the services offered by the ETSF to the scientific community interested on the ab-initio characterization of electron excitations.

Detailed information about the Workshop (registration, deadlines, etc.) can be found in the URL <http://www.tddft.org/ETSF2009>



Welcome to the fourth edition of the ETSF Users' Newsletter. On page 2, you will find the agenda and the User Corner: Alexander Grüneis presents his work on Graphene. Don't miss it! The beamline presented in this issue is brand new: Vibrational Spectroscopy! Last but not least, note that a users' meeting will take place next September in Portugal.

Submission deadline for the Spring evaluation of the ETSF call for proposals: 7th April 2009, 17:00 (CET).

Vibrational Spectroscopy Beamline



"..everything that living things do can be understood in terms of the jiggings and wiggings of atoms.."* R. P. Feynman

This beamline is dedicated to vibrational spectroscopies, such as Infrared absorption and Raman scattering. These two experimental techniques allow to determine the vibrational properties of matter (phonons in solids or molecular vibrations, typically in the 100-5000 cm⁻¹) by analyzing its interaction with light: absorption and scattering of photons.

In Infrared spectroscopy, infrared light over a broad frequencies is passed through a sample. The matter absorbs the light only for some specific frequencies corresponding to the vibrational modes of the system and which fulfill some selection rules (the IR-active

modes). Hence, for these frequencies, the light is attenuated when it passes through the sample. By measuring the intensity of the transmitted light at each frequency, the IR-active modes can be determined.

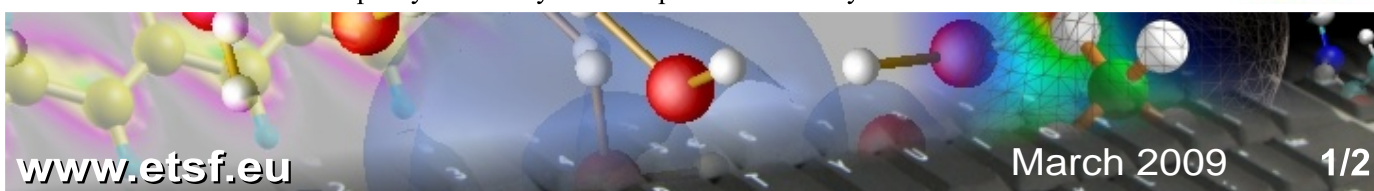
In Raman spectroscopy, a sample is illuminated with a monochromatic light (usually laser beam in the visible, near infrared, or near ultraviolet range). The light interacts (inelastic or Raman scattering) with some specific vibrational modes of the system, which fulfill selection rules that are complementary to IR spectroscopy (Raman-active modes). As a result, the energy of the laser photons (and hence, the frequency of the light) may be shifted up or down by amounts corresponding to the various energies of the vibrational modes of the system.

Beamline Coordinator: Gian-Marco Rignanese
Gian-Marco.Rignanese@uclouvain.be

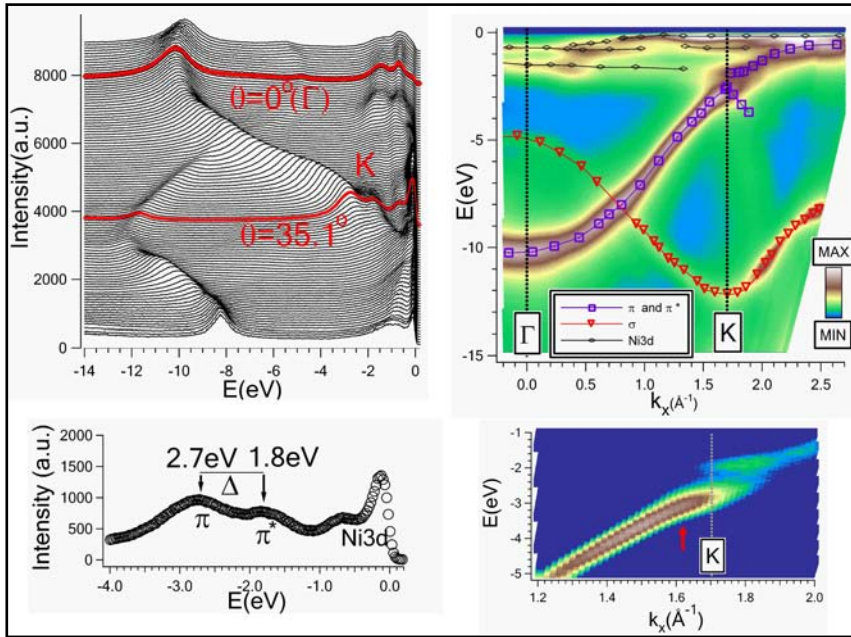
* Feynman, R. P. (1963) Six Easy Pieces (Addison-Wesley, Reading MA), p 59.

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e-infrastructure



User Corner: Graphene



Band-structure of graphene on a Ni(111) surface, measured with ARPES
Phys. Rev. B 77, 193401 (2008)

1) Dr Grüneis, you work on Graphene at the Leibniz-Institut für Festkörper- und Werkstoffforschung in Dresden (Germany). Which scientific problem are you currently working on?

We are currently working on the problem of correlation effects and electron phonon coupling in graphene - a one atom thick layer of carbon. To this end we apply angle resolved photoemission spectroscopy using synchrotron radiation sources.

2) How (and when) did you get in touch with the ETSF?

I got in touch with ETSF in person of Prof. Angel Rubio via one of my collaborators (Prof. T. Pichler). Prof. Rubio and his coworkers, in particular Claudio Attacalio and Ludger Wirtz assisted us in interpreting our experiments and made valuable suggestions for new experiments.

3) What do you expect from this collaboration?

I expect that with our joint experimental and theoretical approach we will be not only able to get a deeper understanding of what we measure in terms of the underlying quantum mechanical processes but also to efficiently plan and select

experimental geometries. This is further evidenced by a recent experiment where we measure phonon dispersion relations in graphene layers: the ETSF suggested particular scattering geometries that allowed us to map phonon dispersions of particular vibrations around a Kohn anomaly.

Alexander Grüneis:

alexander.grueneis@univie.ac.at

ETSF Agenda

24-27 March 2009 ABINIT 2009 - 4th developer workshop, Autrans (France)

7 April 2009 Submission deadline for the Spring evaluation of the ETSF call for proposals

25-29 Mai 2009 Theoretical Spectroscopy Lectures, Zürich (Switzerland)

14-19 Sept. 2009 Ab-initio tools for the characterization of nanostructures, Nanoquanta-ETSF Workshop, Evora (Portugal)