THEORETICAL SPECTROSCOPY

The ETSF Users' Newsletter

September 2011, issue. 8

ETSF

European Theoretical Spectroscopy Facility

Welcome to the eighth edition of the ETSF Users' Newsletter. In this issue, we chat to one of our users about his experiences with the ETSF, and also find out more about the ETSF's Optics Beamline. Don't miss the upcoming events listed on page two.

Submission deadline for the ETSF's Autumn 2011 call for proposals: 25 October, 17:00 (CET).

ETSF-SOLEIL joint call for proposals

A first joint call for proposals with an experimental facility was held in September this year. Users had the opportunity to request both experimental beamtime and theoretical support, when applying for a project with the French Syncrotron, SOLEIL. Use of the SOLEIL synchrotron source offers new perspectives such as scanning imagery on micro- and submicro-metric scales, or monitoring of kinetics in real time, on top of all standard synchrotron techniques (XPS, EXAFS, etc.). More information can be found at:

http://www.synchrotron-soleil.fr/portal/page/portal/Recherche/SUN/GuideUtilisateurs/DemandeTempsFaisceau

Theoretical support will consist of *ab initio* calculations of electronic structure and valence electron spectra (photoemission, inelastic x-ray scattering and/or absorption), training on theory and computer codes, and/or discussion and analysis.

The ETSF's theoretical expertise complements that of SOLEIL's experimental expertise. This call is a first step towards facilitating access to experimental and theoretical services simultaneously. We envisage joint calls with other experimental facilities, in a wider range of topics.

Optics Beamline

Optics Beamline Coordinator
Prof. Olivia Pulci
pulci@roma2.infn.it

The ETSF Optics Beamline (OBL) is dedicated to the *ab-initio* calculations of the optical response of matter. Dielectric functions, absorption spectra, cross-sections, reflectance anisotropy, birefringence, chirality, and second harmonic generation, are quantities that are studied in this beamline.

The OBL has attracted a large interest in the scientific community, as witnessed by the large number of user projects implemented within the beamline. This success can be attributed to the fact that the characterization of materials with outstanding optoelectronic properties represents the first step in the design of novel opto-devices. Indeed, Optical Spectroscopies represent the prime experimental methodology used to investigate the excited state properties of complex materials. Consequently, the applications to the OBL have covered very different areas of the material science community, from nano objects to complex molecular aggregates.

Collaboration between ETSF nodes have made available to the users theoretical and computational tools based on the Many-Body Theory or on the Time-dependent Density Functional Theory.

Optics Beamline, continued …

There are a large variety of projects submitted to the OBL, many of which are in collaboration with experimentalists. It is worth highlighting the modernity of the subjects, ranging from materials for photovoltaics (TiO2, ZnO) to quantum dots, nanowires, surfaces, biomolecules. All projects have been quite successful, leading to numerous publications and an active and prolific interaction within the ETSF nodes.

User Corner: Photoemission of Transition Metal Alloys

Prof. Enrique Ortega is an experimentalist whose focus is on the description of the morphology and the electronic states in nanostructures. We asked him some questions about his project with the ETSF.

How did you hear about the ETSF?

The San Sebastian node is led by an old colleague, Angel Rubio, whose work is highly appreciated. He told me about the ETSF Project and I immediately liked it, and joined from the beginning.

What scientific problem were you working on when you contacted the ETSF?

I was working on two parallel projects, one related to donor/acceptor molecular networks in contact with metal surfaces, and the other one related to two-dimensional binary metallic alloys.

What were you expecting from your collaboration with the ETSF, and what was your experience?

I expected a relatively prompt response to our theoretical needs in the mentioned problems. I got it, my experience is very positive.

What were you able to conclude from the project?

The calculated atomic and electronic properties of a rare-earth alloy (Gd Au2) are in agreement with experimental results employing surface-sensitive techniques [1]. We clarified many complex issues around both problems, and more importantly, we found exotic, new physics out of the theory calculations that are now being explored in both directions, theory and experiment.

[1] M. Corso, *et al.* (2010)."Rare-earth thin-film alloying: a new phase for GdAu2". *Phys. Rev. Lett.* **105**, 016101.

ETSF Agenda

27-30 September 2011 16th ETSF workshop on Electronic Excitations

25 October 2011 Submission deadline for Autumn evaluation of the ETSF call for proposals

4-18 January 2012 5th School & Workshop on "Time-Dependent Density-Functional Theory: Prospects and Applications"

More information about these events at ***www.etsf.eu***