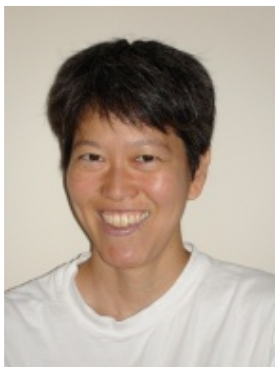


# THEORETICAL SPECTROSCOPY

## *The ETSF Users' Newsletter*

### Introduction to the Chief Executive of ETSF

In August 2009, the ETSF hired its first chief executive, Dr. Anne Matsuura. Dr. Matsuura has joined the ETSF's central node in Louvain-la-Neuve. Prior to coming to the ETSF, she served as a funding agent for university basic research, a Special Assistant for an U.S. Deputy Under Secretary of Defense, and worked for InQTel, a strategic investor in start-up technical companies. Anne's original science training was in highly correlated materials related to high temperature superconductors, and she has experience as an experimentalist at synchrotron sources worldwide.



Anne's role is to improve ETSF publicity, to promote fund-raising, and to attract more corporate users to the ETSF. Her addition to the ETSF administration will strengthen the organization and will help us to chart a course toward a more successful future for the ETSF.

Anne Matsuura: [anne.matsuura@uclouvain.be](mailto:anne.matsuura@uclouvain.be)



Welcome to the fifth edition of the ETSF Users' Newsletter. On page 2, you will find the agenda and the User Corner: Steen Nielsen presents his work on Gas-Phase Ion Spectroscopy. You are also invited to get to know the Energy Loss Spectroscopy Beamline as well as the new ETSF Chief Executive: Dr. Anne Matsuura.

**Submission deadline for the Autumn evaluation of the ETSF call for proposals: 27th October 2009, 17:00 (CET).**

## Energy Loss Spectroscopy Beamline

The Energy Loss Spectroscopy (ELS) Beamline is dedicated to studying, describing and predicting the outcomes of several energy loss experimental techniques, such as Electron Energy Loss (EELS) and Inelastic X-ray Scattering (IXS).

The EELS and the IXS are two very different (electron microscope for EELS; synchrotron radiation for IXS) and yet complementary experimental techniques, in many respects. Energy, momentum, and spatial resolution are different for the two techniques, for instance. However, both EELS and IXS measure the same quantity, the dynamical structure factor  $S(\mathbf{q}, \omega)$ . This quantity is related to the inverse dielectric function  $\epsilon^{-1}(\mathbf{q}, \omega)$ , which is the quantity that is actually calculated via

ab initio theoretical approaches, such as TDDFT or BSE [1].

New topics of the Beamline are represented by: EELS at Surfaces, Coherent IXS and Reflection EELS.

Beamline Coordinator: Francesco Sottile  
[Francesco.Sottile@polytechnique.fr](mailto:Francesco.Sottile@polytechnique.fr)

[1] Comptes Rendus Physique 10, issue 6 - Theoretical Spectroscopy (Ed. Lucia Reining) 2009.

The ETSF is partly funded by the European Community

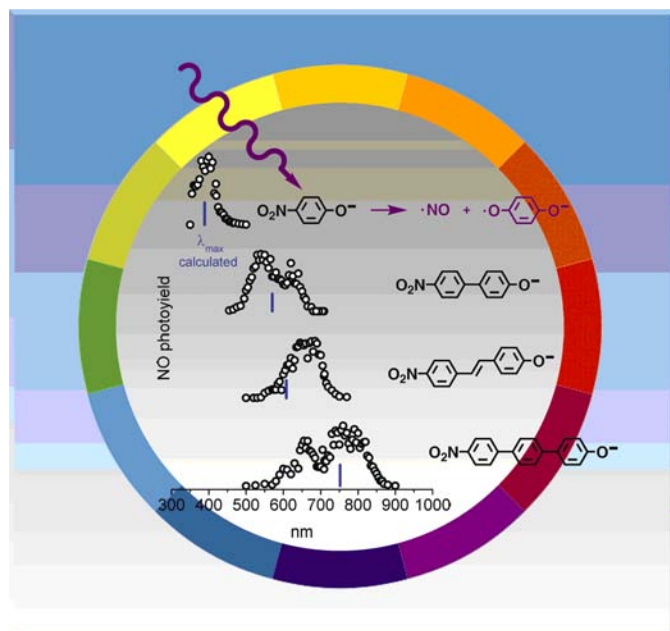
e-infrastructure



## User Corner: Gas-Phase Ion Spectroscopy

1) Dr Nielsen, you work on gas-phase spectroscopy at the Department of Physics and Astronomy, Aarhus University (Denmark). Which scientific problem are you currently working on?

In my group we study the influence of a chemical environment on the electronic structure of chromophores, this could be solvent molecules or amino acids within a hydrophobic protein pocket. To obtain this information, we record absorption spectra of isolated chromophore ions in vacuo. An important aspect is to compare with excited states calculations and in this way benchmark theory. In a recent study we looked at some charge-transfer species with varying length between the donor and acceptor groups and found that theory was right on (see figure).



**From blue to red:** While four  $\pi$ -conjugated nitrophenolates absorb within a relatively narrow region in solution, they cover the entire visible spectrum when isolated in vacuo. The work combines gas- and solution-phase spectroscopy and provides the first benchmark of theoretical excitation energies for nitrophenolates (blue lines are CC2-calculated values).

M.-B.S. Kirketerp et al., Chem. Phys. Chem. 2009, 10, 1207 – 1209.

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

This was from my collaboration with Prof. Angel Rubio (San Sebastian). I believe it was spring this year.

3) What do you expect from your ETSF user project?

I think that the collaboration will be significantly strengthened, and that we will be able to develop better and better models to describe the excited states of molecular ions. Theory and experiments should go hand and hand together, and the ETSF is an excellent tool to allow for this.

4) You were invited to give a talk at the ETSF Workshop [1]. As an experimentalist, what did you gain from it?

Most of the conferences I go to are dominated by experimentalists so it was very fruitful to meet other people and learn about some, to me at least, new theoretical methods. As an example, I have for a long time considered to study the chromophores of fireflies and realized at the meeting that work is currently being undertaken by theorists to understand both emission and absorption properties. No reason to wait with experiments!

Steen Brøndsted Nielsen: [sbn@phys.au.dk](mailto:sbn@phys.au.dk)

[1] ETSF Workshop on Electronic Excitations 2009, Evora (Portugal), September 14-19 2009

### ETSF Agenda

**27 October 2009** Submission deadline for the Autumn evaluation of the ETSF call for proposals

**2-15 January 2010** Time-Dependent Density-Functional Theory: Prospects and Applications 4th International Workshop and School, Benasque (Spain)