

# Recent advances in DFT and TDDFT electronic structure calculations

Hanasaari, Helsinki

14.11.2011

## Venue:

Hanasaari, Meeting Room Solveig  
Hanasaarenranta 5, 02100 Espoo  
[www.hanaholmen.fi](http://www.hanaholmen.fi)

## Program:

12:00-13:00:	Lunch at Restaurant Johannes	
13:00-13:15:	Opening (Risto Nieminen, Martti Puska)	
13:15-13:45:	Jens Jørgen Mortensen	GPAW: present status and development plans
13:45-14:15:	Jussi Enkovaara	Parallelization in GPAW
14:15-14:45:	Ari Ojanperä	Nonadiabatic electron-ion dynamics within the projector augmented-wave method
14:45-15:15:	Lauri Lehtovaara	Attosecond dynamics in small metal clusters
15:15-15:45:	Discussion session	
15:45-16:15:	Coffee break	
16:15-16:45:	Hannes Jonsson	Self-interaction corrected functionals
16:45-17:15:	Olga Acevedo-Lopez	Simulation and modeling of protected cluster optical properties
17:15-17:45:	Arto Sakko	Inelastic x-ray scattering from molecules
17:45-18:30:	Discussion session	
18:30-21:00:	Sauna and Refreshments	

## Registration:

Please send an e-mail with subject "TDDFT Workshop 2011" to [arto.sakko@aalto.fi](mailto:arto.sakko@aalto.fi)

Please inform us on any dietary restrictions in the e-mail.

Deadline for the registration is 4.11.2011.