

Report on the users and developers meeting at the Technical University of Denmark, May 21-23, 2013

Electronic structure calculations with the GPAW code



Figure 1: Sponsored by psi-k (<http://www.psi-k.org/>)

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What is GPAW

GPAW is a free software electronic structure code written by a community of developers distributed over most parts of the world.

Summary of meeting

The meeting started out with two days of presentations about what people are doing with the GPAW electronic structure code followed by one day of technical discussions mainly for current (and future) developers.

It was great opportunity to bring together all the people that normally only interact via email, irc and conference calls. Everybody could learn from each other and discuss future work face to face.

We managed to make video recording of all talks. Videos and slides are available from our web-page:

<https://wiki.fysik.dtu.dk/gpaw/devel/workshop.html>

Scientific Organizers

- Kristian S. Thygesen, Department of Physics, DTU
- Jens Jørgen Mortensen, Department of Physics, DTU
- Jussi Enkovaara, Aalto University
- Marti Puska, Aalto University

Administrative Organizers

- Marianne Ærsøe, Department of Physics, DTU
- Marcin Dulak, Department of Physics, DTU

Invited speakers

- Ask Hjorth Larsen, University of the Basque Country
- Samuli Hakala, Aalto University
- Bjørk Hammer, Aarhus University
- Hannes Jónsson, University of Iceland
- Per Hyldgaard, Chalmers University of Technology
- Thomas Olsen, DTU Fysik
- Mikael Kuisma, Tampere University of Technology
- Jun Yan, SUNCAT
- Angel Rubio, University of the Basque Country

- Michael Walter, University of Freiburg
- Lauri Lehtovaara, University of Jyväskylä
- Ari Ojanperä, Aalto University

Program

Tuesday (May 21)

10:00	Kristian Thygesen	Welcome
10:00	Jussi Enkovaara	Overview of GPAW
10:30	Jens Jørgen Mortensen	Short history of GPAW and latest news about PAW setups
11:00	Ask Hjorth Larsen	LCAO in GPAW
11:30	Samuli Hakala	Multi-GPU Accelerated Large Scale Electronic Structure Calculations
12:00		<i>Lunch</i>
13:30	Henrik H. Kristoffersen	Simple methods for photo reaction modeling
13:50	Lasse B. Vilhelmsen	Automated Two Step Structure Prediction within GPAW
14:10	Bjørk Hammer	Challenges with the currently (correctly) implemented NEB-method. Should ASE revert to the original more robust NEB-formulation with springs?
14:30	Jess Wellendorff	Exchange-correlation functionals with error estimation
15:00	Hannes Jónsson	Orbital density dependent functionals
15:30		<i>Coffee</i>
16:00	Per Hyldgaard	Electron response in the Rutgers-Chalmers van der Waals density Functionals
16:30	Thomas Olsen	Extending the random phase approximation with renormalized adiabatic exchange kernels
17:00	Mikael Kuisma	Spin-Polarized GLLB-SC potential and efficient real time LCAO-TDDFT for large systems
18:00		<i>Barbecue</i>

Wednesday (May 22)

9:00	Jun Yan	Plasmon, exciton and RPA correlation energy: implementations and applications based on linear density response function
9:30	Arto Sakko, Tuomas Rossi	Combining TDDFT and classical electrodynamics simulations for plasmonics

10:00	Falco Hüser	The GW approximation in GPAW
10:30		<i>Coffee</i>
11:00	Angel Rubio	Time-dependent density functional theory for non-linear phenomena in solids and nanostructures: fundamentals and applications
11:30	Michael Walter	Extensions to GPAW: From polarizable environments to excited state properties
12:00		<i>Lunch</i>
13:00	Lauri Lehtovaara	Au ₄₀ (SR) ₂₄ Cluster as a Chiral Dimer of 8-Electron Superatoms: Structure and Optical Properties
13:30	Ivano E. Castelli	Computational screening of materials for water splitting
14:00		<i>Coffee</i>
14:15	Martti Puska	Non-adiabatic electron-ion dynamics
14:45	Ari Ojanperä	Applications of Ehrenfest dynamics: from excited state evolution of protected gold clusters to stopping of high-energy ions in graphene

Thursday (May 23)

Activities for GPAW developers:

- Coordination of code development and discussions about the future: Quick tour of ongoing projects --- what's the current status?
- Introduction to Sphinx and reStructuredText
- Introduction to testing of GPAW
- Hands on: Write new documentation/tutorials and how to make sure they stay up to date
- *Lunch*
- Status of unmerged branches:
 - rpa-gpu-expt
 - cuda
 - lcaotddft
 - lrtddft_indexed
 - aep1
 - libxc1.2.0
- Questions open for discussion:
 - When do we drop support for Python 2.4 and 2.5?
 - Strategy for porting GPAW to Python 3?

- Switch from SVN to Bazaar and Launchpad?
- Hands on: Write new documentation/tutorials --- continued
- Presentations of today's work and wrap up