

**Report on the CECAM/Psi-k Workshop**  
**“Density Functional Theory: Learning from the past, looking to the future”**  
**Magnus-Haus, Berlin, Germany**  
**July 2-5, 2013**

**Organizers:**

- Attila Cangi, Max-Planck Institute for Microstructure Physics, Halle, Germany
- Stefan Kurth, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain, and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
- Neepa Maitra, Hunter College, CUNY, New York, USA
- Antonio Sanna, Max-Planck Institute for Microstructure Physics, Halle, Germany
- Sangeeta Sharma, Max-Planck Institute for Microstructure Physics, Halle, Germany
- Carsten Ullrich, University of Missouri, Columbia, USA

**Summary of the workshop**

Over the last decades, density functional theory (DFT) has had a profound impact in many fields of science. Its balance between reasonable accuracy and modest computational cost has made DFT the method of choice for calculating the electronic structure of materials. The success of DFT hinges on the availability of accurate approximations to the exchange-correlation functional. While tremendous progress has been made, there are still limitations of the existing functionals, and no universal consensus exists on how to achieve systematic improvement. This problem also concerns the extensions of DFT such as the time-dependent DFT (TDDFT), which has been widely used to calculate excitation spectra of molecules and solids.

While nowadays DFT workshops very often present advances in computation and applications to particular systems of interest, the main focus of this workshop was on the fundamental questions of both DFT and TDDFT. The topics covered ranged from the development of new functionals, lessons learned from simple model systems, to extensions into new realms of the theory. Another aim was to stimulate discussions if and how experiences gained from other methods such as many-body perturbation theory or reduced density matrix functional theory can be useful in the construction of density functionals.

**Scientific content and discussions at the workshop**

The aim of this workshop was to identify and discuss key areas and directions of research in the fundamentals of density-functional theory (DFT) and time-dependent density-functional theory (TDDFT). The following questions were addressed:

- How can we construct better exchange-correlation functionals for ground-state DFT? To go beyond the standard local and semilocal (gradient-corrected) functionals, several avenues were discussed: using the strong-interaction limit as reference system to construct functionals for strongly correlated systems, constructing correlation functionals based on multideterminantal reference states, using constrained interpolation schemes between known limits of exactly solvable reference systems, leading-order corrections to the local-density approximation using semiclassical expansion techniques, and constructing correlation functionals from response theory (using the so-called adiabatic-connection fluctuation-dissipation theorem).
- How can we improve DFT’s capabilities to describe van der Waals interactions? Several promising approaches were discussed: quantum continuum mechanics, insights from resummation of van der

Waals coefficients for certain model systems, or going beyond DFT and using the reduced density matrix as basic variable to formulate the theory.

- Several methods beyond DFT were discussed, and the question was asked how we can learn from these methods and how they help us to improve our current approximations used in DFT. The following methods were discussed: reduced density matrix functional theory, the so-called LDA+U scheme (which combines standard DFT with Hubbard-type Hamiltonians for those parts of the system that are strongly correlated), the quantum Monte Carlo approach, stochastic theory, and wave-function theory.
- In TDDFT, solidifications and extensions of the formal framework were discussed, such as finding new fixed-point proofs of the basic existence theorems which do not rely on Taylor expansion of densities or potentials, and extending the applicability of TDDFT to systems where the electromagnetic field is quantized, or where thermoelectric processes can occur.
- Other discussions of TDDFT concerned questions of how we can use the theory to describe challenging situations such as Rabi oscillations, excitons in solids, or nanoscale conductance. This requires dynamical exchange-correlation functionals which are memory-dependent, have a proper long spatial range, and exhibit discontinuities with respect to changes in particle number. Among the promising new developments discussed was a new extension of the ELK electronic structure code which allows real-time solution of the time-dependent Kohn-Sham equations in a solid, driven by strong laser fields.

Four important scientific advances required in the areas of DFT and TDDFT in the next few years, following the discussions in this workshop, can be identified as follows:

1. Develop an accurate and reliable density-functional approach to treat systems with strong dynamical correlation, such as molecules with stretched bonds, which ensures that molecules dissociate correctly.
2. Develop an accurate and computationally efficient density-functional description of van der Waals interactions which is universally suitable for finite and extended systems.
3. Develop exchange-correlation functionals for TDDFT beyond the adiabatic approximation, which can treat multiple excitations, excitonic Rydberg series, and other intrinsically nonadiabatic processes.
4. Develop practical DFT and TDDFT approaches and explicit exchange-correlation functionals to describe open systems and systems at finite temperatures. Develop and test (TD)DFT approaches for treating dissipation and find ways of assessing their accuracy.

The computational requirements for each of these four problems vary very much and depend on the size of the systems under consideration. However, desktop and departmental computers should be sufficient for most applications. The whole point of DFT and TDDFT is computational efficiency as compared to other, more expensive methods; therefore, supercomputers will rarely be an issue.

### **Assessment of the results and impact of the workshop**

The workshop brought together most of the leading experts working on the theoretical foundations of DFT and TDDFT. The results presented showed the tremendous progress which has been made in the field over the last decades. Just to mention one example: it was impressive to see that DFT methods based on the adiabatic-connection fluctuation-dissipation theorem can now reach an accuracy for thermochemical quantities similar or even superior to that of the most sophisticated wavefunction-based methods of quantum chemistry. At the same time, new topics for (TD)DFT were explored in several talks such as, e.g., the incorporation of quantized electromagnetic fields in a DFT framework or the extension towards the description of thermoelectric phenomena.

We have received a lot of positive feedback from the participants on both the form and the scope of the workshop. Participants were particularly positive about the line-up of well-known speakers as well as the breadth of the topics covered during the workshop. The usefulness of this kind of workshop was

generally agreed upon and further editions in the future will certainly be appreciated by the community.

**Annex**

- Program of the workshop. Two last-minute cancellations of invited speakers (Prof. Mark Casida, Prof. Lucia Reining) are not reflected in the program.
- List of participants



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## Density Functional Theory: learning from the past, looking to the future

July 2, 2013 to July 5, 2013

Location : Magnus-Haus, Am Kupfergraben 7, Berlin, Germany

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### Day 1 - July, 2nd 2013

Welcome

- 14:00 to 14:15 - Welcome and Introduction

Fundamentals and Functional Development in Ground-State DFT

- 14:15 to 14:45 - **Samuel B. Trickey**  
Fast ab initio MD with Non-empirical Orbital-free Density Functionals
- 14:45 to 15:15 - **John F. Dobson**  
A new 3rd-rung correlation energy functional based on Quantum Continuum Mechanics: application to Van der Waals forces.
- 15:15 to 15:45 - **Andreas Savin**  
Correcting density functional models with system-dependent constraints

Coffee Break

- 15:45 to 16:15 - Coffee Break

Fundamentals and Functional Development in Ground-State DFT

- 16:15 to 16:45 - **Kieron Burke**  
Systematic non-empirical derivation of density functional approximations
- 16:45 to 17:15 - **Paola Gori-Giorgi**  
Strong correlation in Kohn-Sham density functional theory
- 17:15 to 17:45 - **Axel Becke**  
Two-Determinant Mixing with a Strong-Correlation Density Functional
- 17:45 to 18:15 - **Klaus Capelle**  
Construction of density functionals by constrained interpolation

Poster Session and Welcome Reception

- 18:30 to 22:00 - Poster Session

### Day 2 - July, 3rd 2013

New Progress in Old Challenges: Functional Development and Applications

- 09:00 to 09:30 - **John P. Perdew**  
Van der Waals Interaction as a Summable Asymptotic Series
- 09:30 to 10:00 - **Adrienn Ruzsinszky**  
van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom
- 10:00 to 10:30 - **Michiel Sprik**  
Water is an oxide: Caution when ionizing

Coffee Break

- 10:30 to 11:00 - Coffee Break

New Progress in Old Challenges: Functional Development and Applications

- 11:00 to 11:30 - **Matthias Scheffler**  
Thermodynamics and Statistical Mechanics from First Principles for Surfaces and Interfaces: Theoretical Challenges, Concepts, and Insights
- 11:30 to 12:00 - **Andrea Floris**  
DFT+U-based Density Functional Perturbation Theory: Applications to MnO, NiO

Lunch Break

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- 12:00 to 13:30 - Lunch

Beyond DFT (many-body, density-matrix, etc.)

- 13:30 to 14:00 - **Evert Jan BAERENDS**  
Density Matrix Theory of Van der Waals Interactions
- 14:00 to 14:30 - **Roi Baer**  
Self-averaging stochastic Kohn-Sham density functional theory MP2 and RPA extensions
- 14:30 to 15:00 - **Gustavo Scuseria**  
Orbital Functionals from Wavefunction Theory

Coffee Break

- 15:00 to 15:30 - Coffee Break

Beyond DFT (many-body, density-matrix, etc.)

- 15:30 to 16:00 - **Nektarios Lathiotakis**  
Local Effective Potentials with Correct Asymptotic Behavior in DFT and Reduced-Density-Matrix-Functional Theory
- 16:00 to 16:30 - **Lucia Reining**  
Density Functional and Many-Body Perturbation Theory approaches: learning from each other

### Day 3 - July, 4th 2013

Ground-state Energies and Excitation Spectra from Linear Response TDDFT

- 09:00 to 09:30 - **Weitao Yang**  
Exchange-correlation energies from response properties
- 09:30 to 10:00 - **Andreas Goerling**  
Correlation Functionals via the Adiabatic-Connection Fluctuation-Dissipation Theorem Boosting Accuracy and Applicability of Density-Functional Methods
- 10:00 to 10:30 - **Mark Casida**  
TBA

Coffee Break

- 10:30 to 11:00 - Coffee Break

Ground-state Energies and Excitation Spectra from Linear Response TDDFT

- 11:00 to 11:30 - **Eberhard K.U. Gross**  
What's the right potential acting on the electrons when the nuclei are not clamped?
- 11:30 to 12:00 - **John Kay Dewhurst**  
Describing the interaction of light and matter beyond ALDA

Lunch Break

- 12:00 to 13:30 - Lunch

TDDFT for Nonlinear and Time-Resolved Phenomena

- 13:30 to 14:00 - **Angel Rubio**  
A TDDFT perspective on nonlinear electronic processes: optics, photoemission and resonant tunneling
- 14:00 to 14:30 - **Nicole Helbig**  
Describing Rabi Oscillations in TDDFT: The Importance of Memory
- 14:30 to 15:00 - **Stephan Kuemmel**  
Derivative discontinuity, nonlocality of the exchange-correlation kernel, and the power of learning from the past

Coffee Break

- 15:00 to 15:30 - Coffee Break

TDDFT for Nonlinear and Time-Resolved Phenomena

- 15:30 to 16:00 - **Robert van Leeuwen**  
Time-dependent density functional theory: the Runge-Gross mapping, initial state dependence and memory
- 16:00 to 16:30 - **Gianluca Stefanucci**  
Dynamical correction to Kohn-Sham conductances from static density functional theory

Conference Dinner

- 20:00 to 23:00 - Social Dinner

### Day 4 - July, 5th 2013

Extensions of (TD)DFT into New Realms

- 09:00 to 09:30 - **Giovanni Vignale**

- 09:30 to 10:00 - **Ilya Tokatly**  
Density-Functional Theory of Thermoelectric Phenomena  
Time-Dependent Density Functional Theory for Many-Electron Systems  
Interacting with Photons: TDDFT for cavity-QED
- 10:00 to 10:30 - **Heiko Appel**  
Intra-system derivative discontinuities in static DFT and correlated photon-electron wavefunctions in cavity QED

**Coffee Break**

- 10:30 to 11:00 - Coffee Break

**Extensions of (TD)DFT into New Realms**

- 11:00 to 11:30 - **Ali Alavi**  
Quantum Monte Carlo approach to Full CI quantum chemistry
- 11:30 to 12:00 - **Giovanni Ciccotti**  
A pseudo-quantum Description of Classical Vacancy Diffusion in Crystals
- 12:00 to 12:30 - **Walter Kohn**  
A World Powered Predominantly by Solar and Wind Energy?

**Closing Word**

- 12:30 to 12:45 - Closing Word

**CECAM - Centre Européen de Calcul Atomique et Moléculaire**  
**Ecole Polytechnique Fédérale de Lausanne, Batochime (BCH), 1015 Lausanne, Switzerland**



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### Australia

- John F. Dobson (**invited speaker**) (Griffith University, Nathan)

### Austria

- Michael Ruggenthaler (Institute for Theoretical Physics, University of Innsbruck)

### Brazil

- Klaus Capelle (**invited speaker**) (Federal University of ABC, Santo André)

### Canada

- Axel Becke (**invited speaker**) (Dalhousie University, Halifax)

### Finland

- Javad Hashemi (University of Helsinki)
- Robert van Leeuwen (**invited speaker**) (University of Jyväskylä)

### France

- SIWAR CHIBANI (chemistry)
- Ymène Houari (University of Nantes)
- Andreas Savin (**invited speaker**) (University Pierre and Marie Curie, Paris)

### Germany

- Ali Abedi Khaledi (MPI Halle)
- Federica Agostini (Max Planck Institute of Microstructure Physics, Halle)
- Heiko Appel (**invited speaker**) (Fritz Haber Institute of the Max Planck Society (FHI), Berlin)
- Markus Betzinger (Forschungszentrum Juelich)
- John Kay Dewhurst (**invited speaker**) (Max Planck Institute of Microstructure Physics, Halle)
- Tanja Dimitrov (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
- Peter Elliott (Max Planck Institute of Microstructure Physics)
- Frank Essenberg (MPI für Mikrostrukturphysik Halle (Saale))
- Kati Finzel (Max-Planck-Institute for Chemical Physics of Solids)
- Johannes Flick (Fritz Haber Institute of the Max Planck Society (FHI), Berlin)
- Sebastian Frank (Max Planck Institute of Microstructure Physics, Halle)
- Henning Glawe (MPI Halle)
- Andreas Goerling (**invited speaker**) (University of Erlangen-Nuremberg)

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- Eberhard K.U. Gross (**invited speaker**) (*Max Planck Institute of Microstructure Physics, Halle*)
- Nicole Helbig (**invited speaker**) (*Forschungszentrum Juelich*)
- Kim Julia Hintze (*Mulliken Center for Theoretical Chemistry, University of Bonn*)
- Elham Khosravi (*HU Berlin, Institut für Physik, Newtonstr. 15*)
- Stephan Kuemmel (**invited speaker**)
- Manfred Lein (*Institut fuer Theoretische Physik, Universitaet Hannover, Germany*)
- Andreas Linscheid (*Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle*)
- Michael Lubasch (*Max-Planck-Institute of Quantum Optics*)
- Ingrid Mertig (*Martin-Luther University Halle-Wittenberg*)
- Seung Kyu Min (*Max-Planck-Institut für Mikrostrukturphysik*)
- Sareh Motahari (*Max Planck Institute of Microstructure Physics, Halle, Germany*)
- klaus-robert mueller (*TU Berlin*)
- Mariana Odashima (*Max-Planck-Institut für Mikrostrukturphysik*)
- Yang Peng (*Fritz Haber Institute of the Max Planck Society (FHI), Berlin*)
- Erich Runge (*Technical University Ilmenau, Ilmenau, Germany*)
- Marie-Christine Runkel (*Mulliken Center for Theoretical Chemistry, University of Bonn*)
- Matthias Scheffler (**invited speaker**) (*Fritz Haber Institute of the Max Planck Society (FHI), Berlin*)
- Yasumitsu Suzuki (*MPI Halle*)
- Falk Tandetzky (*Max Plank Institute of Microstructure Physics*)
- Walter Tarantino (*Max Planck Institute of Microstructure Physics*)
- Angelica Zacarias (*Freie Universitaet Berlin*)

## Greece

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- Nektarios Lathiotakis (**invited speaker**) (*Theoretical and Physical Chemistry Institute Athens*)

## Hungary

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- Gabor Csonka (*Budapest University of Technology*)

## Israel

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- Roi Baer (**invited speaker**) (*Hebrew University of Jerusalem*)

## Italy

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- Giovanni Ciccotti (**invited speaker**) (*University of Rome "La Sapienza"*)
- Gianluca Stefanucci (**invited speaker**) (*University of Rome, Tor Vergata, Italy*)

## The Netherlands

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- Evert Jan BAERENDS (**invited speaker**) (*VU university amsterdam + Pohang Un. of Science and Techn., South=Korea*)
- Klaas Giesbertz (*VU University*)
- Paola Gori-Giorgi (**invited speaker**) (*Vrije Universiteit Amsterdam*)
- Francesc Malet Giralt (*Department of Theoretical Chemistry, Faculty of Sciences, Vrije Universiteit Amsterdam*)
- Andre Mirtschink (*Vrije Universiteit Amsterdam*)

## Spain

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- Mehdi Farzanehpour (*University of Basque country, Nano bio spectroscopy group*)
- Camilla Pellegrini (*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Centro de Física de Materiales, Universidad del País Vasco UPV/EHU*)
- Angel Rubio (**invited speaker**) (*University of the Basque Country, San Sebastian*)
- Ilya Tokatly (**invited speaker**) (*Universidad del País Vasco UPV/EHU, San Sebastian*)
- Perla Wahnon (*Universidad Politecnica de Madrid*)

## Sweden

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- [Daniel Karlsson](#) (*Lund University*)

### United Kingdom

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- [Ali Alavi](#) (**invited speaker**) (*University of Cambridge*)
- [Andrea Floris](#) (**invited speaker**) (*King's College London*)
- [Michiel Sprik](#) (**invited speaker**) (*University of Cambridge*)
- [Hassan Tahini](#) (*Imperial College London*)

### USA

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- [Kieron Burke](#) (**invited speaker**) (*University of California at Irvine*)
- [Florian Eich](#) (*University of Missouri*)
- [Johanna Ildemar Fuks](#) (*Hunter College City University New York*)
- [Walter Kohn](#) (**invited speaker**)
- [Ann Mattsson](#) (*Sandia National Laboratories*)
- [John P. Perdew](#) (**invited speaker**) (*Department of Physics, Tulane U.*)
- [Stefano Pittalis](#) (*University of California, Irvine*)
- [Adrienn Ruzsinszky](#) (**invited speaker**) (*Department of Physics, Temple University*)
- [Gustavo Scuseria](#) (**invited speaker**) (*Rice University, Houston*)
- [Justin Smith](#) (*University of California, Irvine*)
- [Samuel B. Trickey](#) (**invited speaker**) (*University of Florida*)
- [Giovanni Vignale](#) (**invited speaker**) (*University of Missouri*)
- [Lucas Wagner](#) (*University of California, Irvine*)
- [John Wills](#) (*Los Alamos National Laboratories*)
- [Weitao Yang](#) (**invited speaker**) (*Department of Chemistry, Duke University*)

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