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$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{N}\nabla_{\mathbf{r}_i}^2 + \frac{1}{2}\sum_{i}^{N}\sum_{j\neq i}^{N}\frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i-\mathbf{r}_j|} + \sum_{i}^{N} v(\mathbf{r}_i)$$

$$T_{\mathrm{W}}(\rho) = \frac{1}{2}\int_{\mathbb{R}^3}\left|\nabla\sqrt{\rho(\mathbf{x})}\right|^2 \mathrm{d}\mathbf{x}$$

$$\mathcal{F}^{\varepsilon}(\rho) = \inf_{\sigma}\left\{\mathcal{F}(\sigma) + \frac{1}{2\varepsilon}\|\sigma-\rho\|^2\right\}$$

$$F_{\mathrm{LL}}(\rho) = \inf_{|\psi\rangle\mapsto\rho}\langle\psi|\hat{H}_0|\psi\rangle$$

$$\rho_\psi(\mathbf{x}) = N\int_{\mathbb{R}^{3(N-1)}}|\psi(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2\mathrm{d}\mathbf{x}_2\ldots\mathrm{d}\mathbf{x}_N$$

$$E^{\varepsilon}(v) = \inf_{\rho}\{\mathcal{F}^{\varepsilon}(\rho) + \langle v,\rho\rangle\}$$

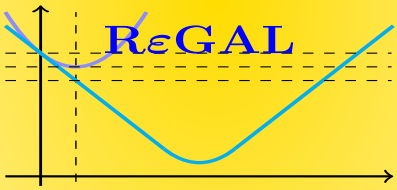
$$E(v) = E^{\varepsilon}(v) + \frac{\varepsilon}{2}\|v\|^2$$

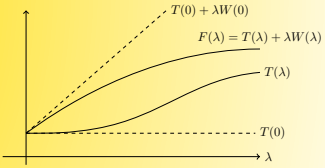
Workshop on the Foundations and Extensions of Density-Functional Theory

$$\mathcal{F}(\rho) = \sup_{v}\{E(v) - \langle v,\rho\rangle\}$$

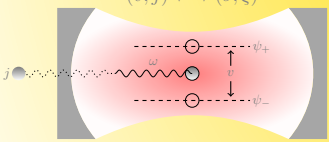
$$E(v) = \inf_{\rho}\{\mathcal{F}(\rho) + \langle v,\rho\rangle\}$$

$$i\hbar\tfrac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{H}|\psi\rangle$$





$$(v,j) \longleftrightarrow (\sigma,\xi)$$



$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$F_{\mathrm{DM}}^{\lambda}(\rho) = \inf_{\Gamma}\mathrm{Tr}\left[(\hat{T}+\lambda\hat{W})\Gamma\right]$$

$$\overline{\partial}_\lambda F_{\mathrm{DM}}^{\lambda}(\rho) \ni \mathrm{Tr}\,\hat{W}\Gamma^{\lambda}$$

$$F_{\mathrm{DM}}^{\lambda}(\rho) = F_{\mathrm{DM}}^{0}(\rho) + \int_0^{\lambda}\mathrm{Tr}\,\hat{W}\Gamma^{\mu}\,\mathrm{d}\mu$$

Oslo

April 20th – 24th, 2026

European Research Council

Established by the European Commission

Workshop on the Foundations and Extensions of Density-Functional Theory

André Laestadius[*,†] and Vebjørn H. Bakkestuen[*,✉]

Pilestredet 35, 0166 Oslo, Norway

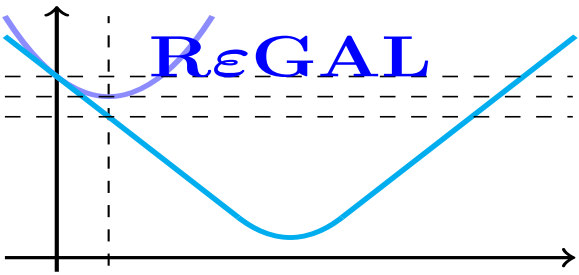
20.04.2026 – 24.04.2026

[*] *Department of Computer Science, Oslo Metropolitan University*

[†] *Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo*

✉ vebjorn.bakkestuen@oslomet.no

https://uni.oslomet.no/regal/workshop-foundations-and-extensions-of-dft/



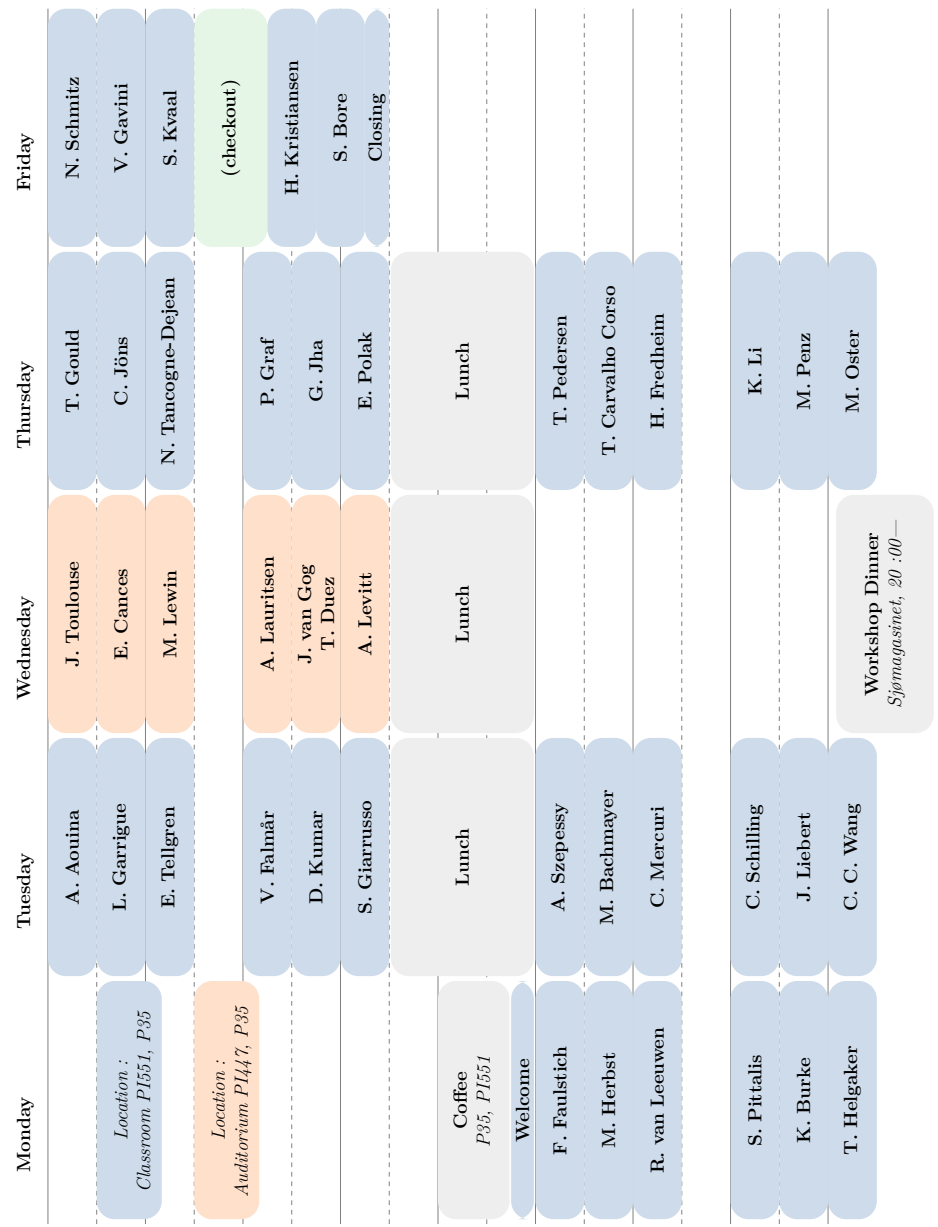
Abstract

The workshop is devoted to the rigorous mathematical analysis and recent theoretical advances in density-functional theory (DFT), a cornerstone of computational quantum chemistry. While DFT has proven remarkably successful in practical applications, many of its core concepts remain mathematically underexplored. A central theme of the workshop will be the inverse Kohn–Sham problem—the task of reconstructing the effective non-interacting Kohn–Sham potential from a given electronic density. A central question is whether this inverse formulation offers a way to analyse the structure of the universal density functional and for evaluating the accuracy of approximate functionals. Despite its fundamental importance, the inverse problem is significantly less studied than the forward Kohn–Sham scheme and presents unique analytical and numerical challenges, including issues of existence, uniqueness, and stability of solutions. Additionally, the workshop will cover a range of other topics within the analysis of DFT, including foundational questions, extensions, functional approximation strategies, regularisation approaches, and numerical methods. The final composition of the program will be shaped by the interests and expertise of the confirmed participants. The workshop aims at bringing together researchers working on these and adjacent subjects in order to advance the applicability of DFT in both novel and established domains.

Contents

Schedule

	Time	Location	Event	Chair
Mon	13:00–13:45	PI551	Coffee & mingle	
	13:45–14:00	PI551	Welcome	
	14:00–17:30	PI551	Talks	Laestadius
Tue	09:00–12:30	PI551	Talks	Bakkestuen
	12:30–14:00		Lunch	
	14:00–17:30	PI551	Talks	Tellgren
Wed	09:00–12:30	PI447	Talks	Penz
	12:30		Group photo	
	12:30–14:00		Lunch	
	20:00–	Sjømagasinet	Dinner	
Thu	09:00–12:30	PI551	Talks	Pittalis
	12:30–14:00		Lunch	
	14:00–17:30	PI551	Talks	Helgaker
Fri	09:00–12:30	PI551	Talks	Faulstich
	12:30–12:45	PI551	Closing	


Monday
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Friday
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17 : 00
A. Aouina
L. Garrigue
E. Tellgren
V. Falmår
D. Kumar
S. Giarrusso
Coffee
P35, P1551
Welcome
F. Faulstich
M. Herbst
R. van Leeuwen
S. Pittalis
K. Burke
T. Helgaker
Location :
Classroom P1551, P35
Location :
Auditorium P1447, P35
J. Toulouse
E. Cances
M. Lewin
A. Lauritsen
J. van Gog
T. Duez
A. Levitt
Lunch
A. Szepessy
M. Bachmayer
C. Mercuri
C. Schilling
J. Liebert
C. C. Wang
T. Gould
C. Jöns
N. Tancogne-Dejean
P. Graf
G. Jha
E. Polak
Lunch
T. Pedersen
T. Carvalho Corso
H. Fredheim
K. Li
M. Penz
M. Oster
Workshop Dinner
Sjømagasinet, 20 :00—
N. Schmitz
V. Gavini
S. Kvaal
(checkout)
H. Kristiansen
S. Bore
Closing

Practicalities

Venue

The workshop will be held at the Pilestredet campus of OsloMet. All lectures, talks, and discussions will take place at *Ellen Gleditschs hus* (P35), Pilestredet 35, 0166 Oslo. Please use the rotating doors facing Holbergs plass as they are unlocked during the day, see Figure 2.1.

The most of the workshop will take place in the classroom PI551, located on the fifth floor in P35. Please see the Mazemap for directions.

The morning session on Wednesday will take place in the auditorium PI447, which is located on the fourth floor in P35. Please see the Mazemap for directions.

Both rooms (PI551 and PI447) are located in the same part of P35, albeit on different floors. To access the rooms, please locate the glass elevators in the large open space directly inside the entrances to P35. Follow the stairs to the 4th or 5th floor, for PI4447 or PI551, respectively. Both rooms are located on the left-hand side when coming up the stairs (right-hand side if you are taking the elevators).

Figure 2.1: View of the entrance to P35 form Holbergs plass.
(Photo: Benjamin A. Ward/OsloMet)

Directions

From the airport by train: Exit at *Nationaltheatret station*, the stop after Oslo Central Station (Oslo S). Then P35 is only short walk away, < 10 min, see Figure 2.2.

From elsewhere in the city: The closest subway station (T-banen) is *Nationaltheatret station*, see Figure 2.2. By bus or tram, the closest station is *Holbergs plass* just outside P35.

Figure 2.2: Directions from *Nationaltheateret station* to *Ellen Gleditschs Hus (P35)*. On foot it takes less than 10 minutes. (Map by Apple)

Lunches & Dinners

The Pilestredet campus is located centrally in Oslo and there is a variety of options for both lunch and dinner. During the workshop there will not be any organised lunches, and all participants are free to explore the local restaurants and cafeterias. Please note that restaurants in Norway generally close a bit earlier than in other countries in Europe. It is not uncommon that the kitchen closes as early as 21:00, but this might vary from restaurant to restaurant.

In addition to restaurants, there are a few options for lunch on campus. Some options are, the *SiO* cafeterias in P32, P35 (a smaller one), and P52 which offer a variety of warm dishes, salads, baguettes etc. Please note that most options are priced by weight, currently at 19.70 NOK per hg., about €17.75 per kg. In addition, *Union167 Fyrhuset* offers a selection of baked goods, sandwiches and freshly baked pizzas, with pizzas raging from €12 to €16.

Workshop Dinner

The workshop dinner will be held on Wednesday the 22nd of April at 20:00. The dinner is included for all participants, but any beverages must be covered by the participants themselves. If you have any allergies or other restrictions that the organisers have not been made aware of, please contact Vebjørn as soon as possible.

The dinner will be held at Sjømagasinet[1] located near the waterfront between *Aker brygge* and *Tjuvhomen*. The restaurant is a 20-25 min walk away from the workshop venue, see Figure 2.3 (next page).

The organisers invite all participants join for a pre-dinner drink before walking to the restaurant. More details will follow during the morning sessions on Wednesday.

[1]Address: Tjuvholmen Allé 14 0252 Oslo. Website: https://www.sjomagasinet.no

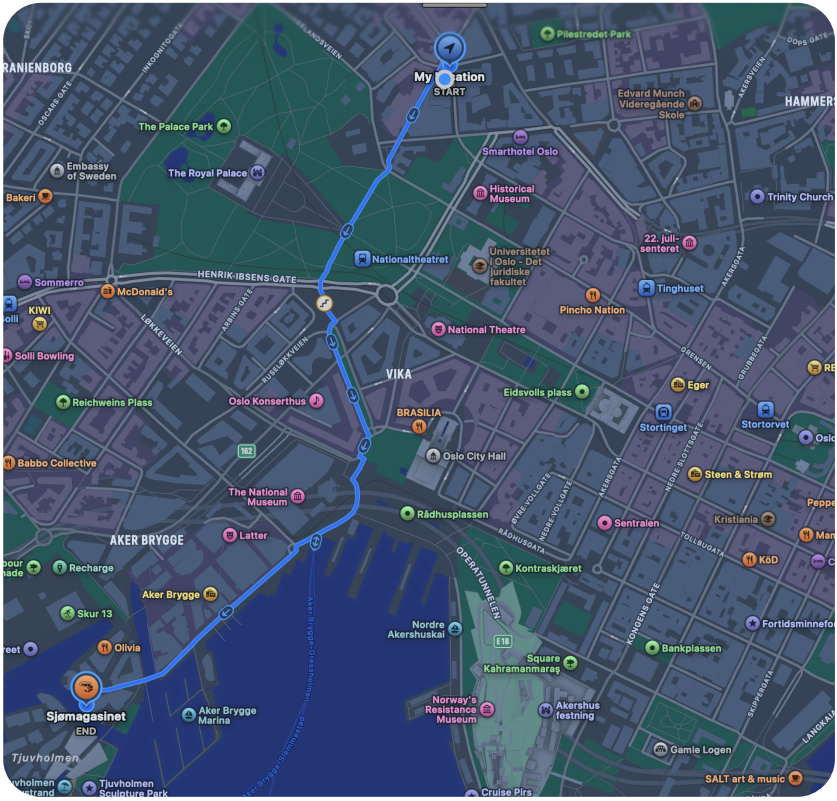

Figure 2.3: Route to Sjømagasinet, the venue of the workshop dinner, from OsloMet. (Map by Apple)

Abstracts

Monday April 20th

From Promise to Practice:
Benchmarking Quantum Chemistry on Quantum Hardware
Fabian Faulstich

We provide a systematic evaluation of the sample-based quantum diagonalization (SQD) method for electronic structure based on the W4-11 thermochemistry dataset, comprising 124 total atomization, 83 bond dissociation, 20 isomerization, 505 heavy-atom transfer, and 13 nucleophilic substitution processes, covering diverse bonding situations and reaction mechanisms. This is the largest study assessing the accuracy and precision of a quantum-hybrid algorithm on a digital quantum device across a variety of molecular systems and chemical reactions, using 16.85 hours on the superconducting quantum processor ibm_rensselaer and 724.22 node hours on the supercomputer AiMOS. To ensure a fair comparison, our study employs commensurate resource allocation for both classical and quantum simulations. Although SQD exhibits large statistical deviations from ground-state reference energies, energy extrapolations yield CCSD-level accuracy. While bond-breaking reactions show a systematic improvement as computational resources increase, nucleophilic substitution or heavy atom transfer reactions do not. The limitations quantified in this manuscript indicate opportunities for improvement in SQD-based algorithms. This work provides a benchmark and community resource for exploring new quantum algorithms and devices, supported by an online benchmark challenge and an open-source Python library for direct comparison.

Basis set error estimation in plane-wave density-functional theory

Michael F. Herbst

An an approximation to the Schrödinger equation practical density-functional theory simulations are inexact due to model, discretisation, and algorithmic choices. Estimates for the corresponding error contributions enable opportunities for error balancing. For example, basis set sizes could be chosen smaller if other error sources (such as the DFT model error) are found dominating, leading to overall cheaper simulations while maintaining the accuracy. Likewise quantitative error estimates in generated DFT data can be employed to inform subsequent machine-learned interatomic potentials of the credibility of each training data point, in this fashion avoiding deterioration of atomic potentials from heterogeneous training data.

For plane-wave-discretised DFT simulations the recent development of perturbation-based error estimates [1] is promising to quantitatively capture the discretisation error without substantial additional cost. In this talk I will review this method and present our recent developments to make this idea usable in practice. This considers the development of theoretically inspired black-box techniques for choosing relevant computational parameters to turn these error estimates into a routinely applicable technique. A systematic benchmark study on a wide range of insulators demonstrates the efficiency of the overall procedure as well as the quality of obtained error estimates for state of the art materials simulations.

[1] E. Cancès, G. Dusson, G. Kemlin, and A. Levitt. *Practical error bounds for properties in plane-wave electronic structure calculations*, SIAM J. Sci. Comput. **44**, B1312 (2022).

Lattice density-functional theory in real and imaginary time

Robert van Leeuwen

We introduce an imaginary-time evolution method [1] to evaluate the pure-state constrained-search functional from density-functional theory formulated on finite lattices. Simultaneously, it yields a potential that produces a prescribed density of an eigenstate. Besides being a computational scheme, this allows one to gain theoretical insights into the density-potential mapping. The method can be generalized to the optimization of the expectation value of a general self-adjoint operator on a finite-dimensional Hilbert space under a finite number of expectation-value constraints for commuting self-adjoint operators. We then consider the case of real-time time-dependent density-functional theory involving external potentials in terms self-adjoint operators that span a Lie-algebra. Finally we address future approaches to density-functional real-time dynamics in more general situations.

[1] M. Penz and R. van Leeuwen, *Constrained search in imaginary time*, Phys. Rev. A **112**, 032815 (2025).

Physical spin torques from exactly constrained exchange-correlation functionals

Stefano Pittalis

Capturing spin dynamics in non-collinear magnetic systems remains challenging within spin-density-functional theory (SDFT), where physical spin torques are tied to spin currents not included among the basic variables. This mismatch leads to spurious exchange–correlation (xc) torques and prevents a consistent treatment of spin–orbit coupling. Here, we present a solution based on spin-current density functional theory (SCDFT) [1]. Exploiting the exact local U(1)×SU(2) invariance of the xc-energy functional — a constraint inaccessible to SDFT — we derive xc-torque relations valid for U(1)×SU(2)-invariant meta-GGAs. These relations ensure that xc torques, while essential for stabilizing non-collinear ground states, do not enter the equation of motion for the spin magnetization. Consequently, the adiabatic spin dynamics depend exclusively on physical spin currents and physical torques. Applications reveal significant deviations from SDFT-based approaches [1-3].

[1] J. K. Desmarais, K. Bencheikh, G. Vignale, and S. Pittalis, *Physical spin torques from exactly constrained exchange-correlation torques*, Phys. Rev. Lett. **136**, 016403 (2026).

[2] J. K. Desmarais, A. Erba, G. Vignale, and S. Pittalis, *Meta-Generalized-Gradient Approximation made Magnetic*, Phys. Rev. Lett. **134**, 106402 (2025).

[3] J. K. Desmarais, J. Maul, B. Civalleri, A. Erba, G. Vignale, and S. Pittalis, *Spin-currents via the gauge-principle for meta-generalized-gradient exchange-correlation functionals*, Phys. Rev. Lett. **132**, 256401 (2024).

Approximate Normalizations for Approximate Density Functionals

Kieron Burke

It seems self-evident that a density functional calculation should be normalized to the number of electrons in the system. I will present multiple examples where the accuracy of the approximate energy is improved (sometimes greatly) by violating this basic principle [1]. In one dimension, the appropriate correction to the normalization is explicitly derived. Beyond one dimension, Weyl asymptotics for energy levels yield these corrections for any cavity. I include speculative examples with Coulomb potentials and the exchange energy of atoms to illustrate possible relevance to realistic calculations.

I will also try to explain the bigger picture: Essentially, finite systems have discrete energy levels, while extended systems do not. The normalization corrections arise from this discrete nature and vary with the boundary conditions.

[1] A. Clay, K. Datchev, W. Miao, A. Wasserman, K. Daas, and K. Burke, *Approximate normalizations for approximate density functionals*, Phys. Rev. Lett **136**, 088002 (2026).

The Four-Way Correspondence of Density-Functional Theory

Trygve Helgaker

Density-functional theory (DFT) is conveniently formulated in the language of convex analysis. From the observation that the ground-state energy $E(v)$ is concave and continuous in the external potential v, Lieb [1] observed that it can be represented in terms of a unique universal density functional $F(\rho)$, convex and lower semi-continuous in the density ρ:

$$E(v) = \inf_{\rho} \left(F(\rho) + (v|\rho) \right),$$
$$F(\rho) = \sup_{v} \left(E(v) - (v|\rho) \right).$$

The energy E and density functional F are said to be conjugate functions, depending on the conjugate variables v and ρ, respectively. The density functional defined in this manner is equivalent to Levy's constrained-search functional when formulated in terms of ensembles [2].

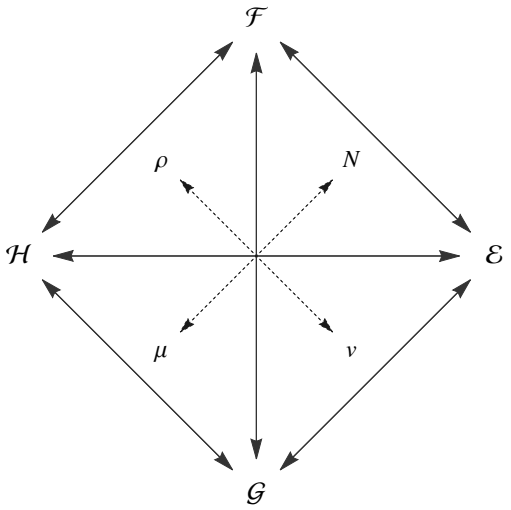

Figure 3.1: Four-way correspondence of DFT

Here, we generalize Lieb's theory to situations where the energy depends on more than one variable, covering the following special cases: (1) *grand-canonical DFT*, where the energy $\mathcal{G}(v, \mu)$ depends also on the chemical potential μ, conjugate to the particle number N; (2) *current-DFT*, where the energy $\mathcal{E}(v, \mathbf{A})$ depends

also on the vector potential $\mathbf{A}$, conjugate to the paramagnetic current density $\mathbf{j}_\mathrm{p}$, and (3) *adiabatic-connection DFT*, where the energy $\mathfrak{E}(v, \lambda)$ depends also on the two-electron interaction strength λ, conjugate to the two-electron expectation value ω. We show how such systems can be treated by a generalization of conjugation to bivariate functions, within the framework of the *four-way correspondence* of convex analysis [3].

Whereas standard DFT sets up a correspondence between two functions E and F, the four-way correspondence sets up a correspondence between four functions: the concave bivariate ground-state energy, the convex bivariate universal density functional, and two semi-universal saddle functions [4]. The four-way correspondence is illustrated in Figure 3.1 for grand-canonical DFT, where the system is described in terms of the conjugate variables v (external potential) and ρ (electron density) and the conjugate variables μ (chemical potential) and N (particle number).

For application of the four-way correspondence in the context of DFT in a magnetic field, see Ref. [5].

[1] E. H. Lieb, Int. J. Quantum Chem. **24**, 243 (1983).

[2] M. Levy, Proc. Natl. Acad. Sci. U.S.A. **76**, 6062 (1979).

[3] R. T. Rockafellar, Pacific J. Math. **25**, 597 (1968).

[4] T. Helgaker, P. Jørgensen, and J. Olsen, Principles of Density Functional Theory, Wiley, in preparation.

[5] S. Reimann, A. Borgoo, E. I. Tellgren, A. M. Teale, and T. Helgaker, J. Chem. Theory Comput. **13**, 4089 (2017).

Tuesday April 21st

Functional and Density-Driven Errors in Density Functional Theory: Quantum Monte Carlo Benchmarks for Solids

Ayoub Aouina

We present a systematic decomposition of density functional approximation errors in solids into functional-driven and density-driven contributions, using quantum Monte Carlo densities of silicon, sodium chloride, and copper as reference. While functional errors dominate in most cases, density-driven errors exceed functional errors by factors of 2–3 for the empirical functionals SOGGA11 and τ-HCTH in the semiconductor and insulator. Material dependence is pronounced: error cancellation occurs in 63% of functionals for silicon but 18% for copper, and only five functionals surpass LDA accuracy in copper even with exact densities. For Si and NaCl, GILL or BECKE exchange combined with PBE, PW91, or P86 correlation achieves near-exact exchange-correlation energies on QMC densities, whereas the metal requires specialized functionals such as PBEsol. Contrary to expectations, several 1990s GGAs outperform many modern meta-GGAs, challenging the notion of systematic improvement along Jacob's ladder, with non-empirical GGAs emerging as the most transferable across material classes. These results provide practical guidance for functional selection and highlight implications for machine learning potential development, where material-dependent error cancellation may compromise transferability.

Mathematical properties of DFT's dual functional, and applications for finding the inverse potential

Louis Garrigue

There are several ways to recover the inverse potential associated with a given target density. We present here an approach based on maximizing the dual problem when the set of potentials is discretized. The advantage of this technique is that it enjoys several favorable mathematical properties, such as coercivity and the absence of local maxima, even in the case of excited states.

Recent results on the regularized Hohenberg–Kohn mapping as well as generalization of the Electron Localization Function

Erik Tellgren

Two themes will be covered. The first is a numerical exploration of a method for approximating the Hohenberg–Kohn (HK) mapping (density-potential inversion) in a controlled manner. The method is based on Moreau-Yosida regularization and puts penalty-term approach on a rigorous footing. It has been implemented in a one-dimensional periodic setting and numerical results provide insight into error propagation through the HK mapping. The second theme is related to a pragmatic unification of meta-GGA functionals and current-density functionals. Within this scheme, tensorial generalizations of the Electron Localization Function (ELF) have been explored. The ELF is essentially an ingredient in meta-GGA functionals that has proven useful for visualization and chemical interpretation.

Limits and Bounds – as Good as it Sounds Regularised Density-Potential Inversion for Periodic Systems

Vegard Falmår

Density-functional theory (DFT) establishes a formally exact framework for describing the electronic structure of atoms, molecules, and materials, but its practical success relies on the accuracy of approximate exchange-correlation functionals. The inverse Kohn–Sham problem – determining the effective Kohn–Sham potential corresponding to a given ground-state density – can provide a deeper understanding of such approximations. While conceptually fundamental, this inverse mapping is notoriously ill-conditioned, particularly in periodic systems. Based on recent work [1], I will present a convex analytic formulation of DFT for periodic systems in arbitrary dimensions employing Moreau–Yosida regularisation of the non-interacting density functional to obtain a robust, regular Hohenberg–Kohn map that is well suited for numerical implementation. The general theory is illustrated with a numerical Hartree–Fock implementation for one-dimensional periodic systems. As a proof of principle, we demonstrate that the local Kohn–Sham potential is able to recover the effects of exact exchange within this scheme. We quantify how errors in the input density propagate through the regularised inversion scheme, combining theoretical bounds with numerical validation. These results establish regularised density-potential inversion as a viable tool for probing exchange-correlation effects in extended systems. The talk will cover more recent work extending the error analysis in [1] as well as results from similar work targeting solid-state systems like bulk silicon, gallium arsenide, and potassium chloride [2].

[1] Bohle, O. M., Lotfigolian, M., Laestadius, A., and Tellgren, E. I., *Regularized density-potential inversion for periodic systems: Application to exact exchange in one dimension*, J. Chem. Phys. **164** (2026) 064104.

[2] Herbst, M. F., Bakkestuen, V. H., and Laestadius, A., *Kohn–Sham inversion with mathematical guarantees*, Phys. Rev. B **111** (2025) 205143.

A direct approach to computing the non-interacting kinetic energy functional

Dharamveer Kumar

The non-interacting kinetic energy functional plays a fundamental role in Density Functional Theory (DFT), yet its explicit form remains unknown for general N-representable electron densities. While it can, in principle, be evaluated through a constrained optimization problem, the associated adjoint problem is not always well posed; even when it is, the corresponding adjoint operator may be singular. To the best of our knowledge, no existing approach in the literature determines the non-interacting kinetic energy functional exactly for a given N-representable density.

In this work, we introduce a variational framework for computing an extension of the non-interacting kinetic energy functional using an exact trigonometric reparametrization of the density. This formulation eliminates the need to solve an adjoint equation. We present a proof-of-concept numerical validation of the variational principle for the special case of one-dimensional Kohn–Sham systems. The approach is general and provides a systematic foundation for computing the non-interacting kinetic energy functional in higher dimensions. In addition, we present an exact kinetic energy functional for certain special cases. This framework may serve as a basis for the development of improved kinetic energy functionals in density functional theory.

From an intrinsic to a fictitious vector potential: exact electron factorization as a route beyond TDDFT

Sara Giarrusso

Starting from the (non-relativistic) time-dependent Schrödinger equation for an N-electron system in the absence of external vector potentials, the exact factorization of the wavefunction into a marginal and a conditional amplitude naturally gives rise to both a scalar and a vector potential with explicit many-body interpretations, extending to the time-dependent domain a construction recently analysed in the static setting [1]. Motivated by the observation that a scalar Kohn–Sham potential cannot in general reproduce an arbitrary physical current density (since the continuity equation constrains only its longitudinal part) and by the expectation that memory-dependent exchange-correlation approximations may be more naturally formulated via a vector potential, I propose an extension of the usual time-dependent density-functional-theory framework in which the non-interacting auxiliary system is subject to both a scalar and a fictitious vector potential. The latter is introduced so that the Kohn–Sham system can match both the time-dependent density and the full current density of the interacting system. Explicit expressions for both scalar and vector potentials emerge from

the exact factorization, and the framework connects naturally to existing ideas in time-dependent current density-functional theory. As the framework is still being developed, contributions and critical feedback from the community are very welcome.

[1] S. Giarrusso, P. Gori-Giorgi, and F. Agostini. *Electronic Vector Potential from the Exact Factorization of a Complex Wavefunction*, ChemPhysChem, **25** (2024) e202400127.

Mean-field molecular dynamics derived from quantum mechanics

Anders Szepessy

Quantum observables determine for instance the stress tensor and heat flux in fluid dynamics. In the talk I will show which properties are used for approximating such quantum observables by classical molecular dynamics and when mean-field molecular dynamics improves the ground state setting in the canonical ensemble.

Block-Sparse Matrix Product States and Eigenvalue Solvers

Markus Bachmayer

Constraining the particle number (or other quantum numbers) in matrix product states leads to a block-sparsity pattern in tensor components that is exploited in many tensor network codes. In this talk, we look at such block-sparsity properties from the perspective of numerical analysis, considering in particular the interaction of the block structure with matrix product operator representations of Hamiltonians in quantum chemistry. We obtain explicit representations of such Hamiltonians operating directly on the block structures, with improved rank bounds under sparsity assumptions on the Hamiltonian coefficients. We the turn to low-rank preconditioned eigensolvers with convergence guarantees and quasi-optimal rank bounds in the context of such block-sparse representations.

Based on joint works with Michael Götte, Sebastian Krämer and Max Pfeffer.

Solutions to nonlinear Schrödinger equations involving Coulombic interactions

Carlo Mercuri

I will discuss two separate classes of nonlinear Schrödinger type equations both involving Coulombic interaction terms, and arising from the quantum many body problem. The first kind of results [1,2], dealing with the multiplicity of stationary solutions, have been recently obtained mainly in collaboration with Kanishka Perera (Florida Institute of Technology) using scaling properties of functionals in an essential way. In the second part of the talk I will instead describe some existence and uniqueness results [3] obtained with collaborators from Eindhoven University of Technology on time dependent Kohn–Sham equations coupled with classical nuclear dynamics.

[1] E. Gloss, C. Mercuri, K. Perera, and B. Ribeiro. *Fractional Schrödinger–Poisson–Slater equations in Coulomb–Sobolev spaces.* arXiv:2511.04829. To appear in the Journal of Geometric Analysis.

[2] Mercuri, C. and Perera, K., *Variational methods for scaled functionals with applications to the Schrödinger–Poisson–Slater equation*, J. Math. Pures Appl. **212** (2026) 103885.

[3] B. Baumeier, O. Çaylak, C. Mercuri, M. Peletier, G. Prokert, and W. Scharpach. *Local existence and uniqueness of solutions to the time-dependent Kohn–Sham equations coupled with classical nuclear dynamics*, J. Math. Anal. Appl. **541** (2025) 128688.

Geometric structure and foundations of functional theories

Christian Schilling

We provide a fresh and more concise perspective on fundamental aspects of functional theories, with an emphasis on one-particle reduced density matrix functional theory (1RDMFT). We introduce the concept of the scope, i.e., the class of systems targeted by the theory, and show that, together with a variational principle for the energy, it gives rise to a corresponding functional theory that is mathematically dual to the scope. This conceptual framework leads to several insights and developments: it highlights the central role of the one-body N-representability problem in 1RDMFT and, using tools from convex analysis, establishes a striking relation between pure- and ensemble-state ground-state functional; drawing on recent results from quantum information theory, it reveals how one-body N-representability constraints shape the universal functional, including the emergence of an exchange force in fermionic systems and a Bose–Einstein force in bosonic systems; and, by replacing the Rayleigh–Ritz variational principle with an ensemble variational principle, it establishes a direct 1RDMFT framework for targeting excited states, made practically feasible through an exact convex relaxation that replaces intricate generalized Pauli constraints with simpler Pauli exclusion principle constraints.

A Symplectic-Geometric Perspective on Functional Theories

Julia Liebert

A range of functional theories in electronic structure can be organized within a common symplectic-geometric framework. The key object is the moment map for a Hamiltonian action of a compact Lie group on projective Hilbert space. After briefly introducing this formalism, we show how the reduced variables and admissible domains of electronic structure functionals arise from suitable symmetry groups and their Lie algebras. We then focus on one-particle reduced density-matrix functional theory (RDMFT), which is from a conceptual point of view particularly well suited to describe the properties of strongly correlated many-electron systems. For spin-adapted RDMFT of spin-1/2 fermions, the natural variable reduces to the orbital 1RDM, which is identified with the moment map for the action of $U(d)$ on the fixed-spin sector of the N-fermion Hilbert space. Its admissible spectra therefore form a moment polytope, and we present new results on the symmetry-adapted pure and ensemble one-body N-representability problem that characterizes this domain.

In the second part of the talk, we introduce an ensemble formalism to target low-lying excited states within RDMFT. We show that the partial trace image of the convex hull of a suitable unitary orbit yields a convex polytope characterizing the set of admissible one-particle reduced density matrices (1RDMs). For these restricted ensembles of fixed spectra, the resulting spectral constraints on the eigenvalues of the 1RDM constitute mixed state generalizations of Pauli's exclusion principle. We then discuss the key structural properties of the facet-defining inequalities of the corresponding moment polytopes and highlight their implications for applications in quantum chemistry.

Boundary forces in generalized density functional theories

Chih-Chun Wang

We introduce and study a general mathematical framework that unifies all variants of ground-state density functional theory on finite-dimensional Hilbert spaces. Within this framework, we focus on a special class, called abelian functional theories, which includes most practically relevant cases, in particular lattice DFT. For these theories, we derive a formula describing the exact behavior of the constrained-search functional near the boundary of its domain. This shows that the universal functional is strongly shaped by the boundary geometry and, in particular, develops a diverging repulsive force when approaching it, thereby generalizing the recently discovered fermionic exchange force and the Bose-Einstein condensation (BEC) force. As a consequence of this formula, we show that for certain systems, such as two-level spin chains, key features of the underlying physical interaction are already encoded in the values of the functional on an arbitrarily small open neighborhood of the extreme points of its domain

Wednesday April 22nd

Geometric Time-Dependent Density Functional Theory

Julien Toulouse

I will introduce a new TDDFT formulation, called geometric TDDFT, which is motivated by the geometric structure of the set of states constrained to have a fixed density. In geometric TDDFT, the time-dependent density is reproduced using an imaginary potential or, equivalently, a self-adjoint non-local operator. I will introduce the corresponding geometric time-dependent Kohn–Sham scheme and highlight some numerical results on model systems. All these aspects will be described in more detail in subsequent talks at the conference.

Joint work with Eric Cancès, Théo Duez, Jari van Gog, Asbjorn B. Lauritsen, and Mathieu Lewin

The geometry of constrained Schrödinger dynamics

Eric Cancès

I will review the geometric foundations of the two standard approaches used to variationally approximate a linear Schrödinger dynamics in a high-dimensional space with an approximate nonlinear dynamics on a lower-dimensional manifold defined by constraints. These two approaches are the time-dependent variational principle and the Dirac-Frenkel principle. They yield identical results when the manifold in question is a Kähler manifold but differ otherwise.

In the new formulation of time-dependent density functional theory (TDDFT) that we propose, we consider a Schrödinger dynamics constrained to have a fixed (time-dependent) density. This type of constraint leads to non-Kählerian manifolds, which explains the discrepancy between the standard formulation of TDDFT (TDKS with a local real effective potential) and our approach (a nonlinear Schrödinger dynamics with a local complex - or nonlocal Hermitian - effective potential).

Joint work with Théo Duez, Jari van Gog, Asbjorn B. Lauritsen, Mathieu Lewin, and Julien Toulouse

A geometric Runge-Gross theorem

Mathieu Lewin

I will present a rigorous Runge-Gross theorem that applies to complex external potentials (with either the real part or the imaginary part fixed). It is an essential ingredient in the new geometric formulation of TDDFT described in other talks at the conference.

Geometric time-dependent density functional theory for lattice systems

Asbjørn Lauritsen

I will review our recent approach to time-dependent density functional theory focusing in particular on the finite-dimensional setting of a (finite) lattice. This is an important model system which still has many of the features of a continuous system, but is mathematically more well-behaved. In particular, we can find more explicit formulas for both the time-dependent Hxc potential V and the new geometric term W reproducing an externally given density $\rho(t)$ and give more concrete conditions for their existence. (In the continuous system, existence of V and W is rather delicate. Uniqueness is the famous Runge–Gross theorem.) Further, I will discuss various Kohn–Sham schemes in this lattice setting illustrating how one can combine existing ideas of (adiabatic) TDDFT with our new geometric approach. If time permits, I will also discuss briefly time-dependent current density functional theory.

Application of Geometric TDDFT to the Hubbard Dimer

Jari van Gog

We apply a geometric formulation of time-dependent density-functional theory (TDDFT) based on the framework developed in Refs. [1, 2] to interacting fermions on the Hubbard dimer. This leads to a time-dependent Kohn–Sham equation with an additional geometric correction, which can be expressed as an imaginary potential. Numerical tests show that this term has a structure qualitatively different from the standard exact time-dependent Kohn–Sham potential. Our results highlight the potential of the geometric framework to motivate alternative approximations, particularly in non-adiabatic regimes.

[1] E. Cancès, T. Duez, J. van Gog, A. Lauritsen, M. Lewin, and J. Toulouse. *Geometric theory of constrained Schrödinger dynamics with application to time-dependent density-functional theory on a finite lattice*, (2026).

[2] E. Cancès, T. Duez, J. van Gog, A. Lauritsen, M. Lewin, and J. Toulouse. *Geometric time-dependent density functional theory*, (2026).

Illustration of the Geometric Principle in TDDFT with a 1D Soft-Coulomb Model

Théo Duez

A geometric formulation of Time-Dependent Density Functional Theory (TDDFT) has recently been introduced in [1, 2]. In order to reproduce a given electronic density, it introduces a purely imaginary potential iW to drive the dynamics, in contrast with the real potential V in standard TDDFT. In this presentation, I will illustrate these ideas using a one-dimensional two-electron soft-Coulomb singlet model, and discuss the main differences between these two formulations as well as their implications for non-adiabatic dynamics.

[1] E. Cancès *et al.*, *Geometric Time-Dependent Density Functional Theory*, arXiv:2601.07724 (2026).

[2] E. Cancès *et al.*, *Geometric theory of constrained Schrödinger dynamics with application to time-dependent density-functional theory on a finite lattice*, arXiv:2601.07719 (2026).

Singular Brillouin zone integrals and spectral properties of periodic crystals

Antoine Levitt

The computation of spectral properties (Green functions, densities of states...) of periodic crystals relies on singular integrals in momentum space. I will describe algorithms to compute these integrals, with applications to solid state physics.

Thursday April 23rd

Ensembles, inversion and some questions they raise

Tim Gould

This talk will survey work on "ensemblisation" and the inverse Kohn–Sham problem in density functional theory (DFT), with a focus on "rigorous" foundations (at physicist level) and their connections to approximations and reality. Both problems reveal limitations of traditional DFT that require new thinking about definitions; and these in turn raise questions for more rigorous formulations of DFT. I'll highlight assumptions and open questions that have been uncovered through this work in the hopes of stimulating more rigorous and/or more general solutions.

Forces, stress, and pressure in density functional theory from the force-balance equation

Nicolas Tancogne-Dejean

The force balance equation represents a formally exact relation connecting the exchange-correlation potential and the exchange-correlation force density, obtained from the kinetic and interaction momentum stress tensors. This framework is valid for both ground-state density functional theory (DFT) as well as time-dependent DFT (TDDFT). It can be used for instance to propose novel functionals that are not derived from an energy, a critical step toward capturing non-adiabatic effects in TDDFT.

In this work, we revisit the link between force and stress densities, in the context of ground-state DFT. We show how the energy density is in fact related to the quantum pressure derived from the force. This work potentially opens new avenues for defining physically meaningful energy densities, based on forces, and relate them to their corresponding potentials, without having to rely to functional differentiation. This also allows us to compare with recent works on the definition of "gauges" for the energy density.

The Virial Relation and the Force-Balance Equation

Christian Jöns

The virial relation provides a fundamental relationship between kinetic and potential energy. In density-functional theory, it offers a useful criterion for assessing the consistency of approximate exchange-correlation functionals. Using the Sturm-Liouville equation, we rewrite the virial relation in terms of the force. Additionally, the equation maps a given force density $\mathbf{F}_{\mathrm{xc}}$ uniquely to both a potential v_{xc} and the virial energy E_{xc}. This unique mapping enables a framework for constructing functionals based on the force density.

On an Attempt to Capture Strong Electron Correlation at Mean-Field Computational Cost

Paul Graf

We introduce and examine i-DMFT, a recently proposed variant of one-particle reduced density matrix functional theory. It augments the Hartree-Fock (HF) functional by approximating the missing correlation energy via a conjectured linear relation with the nonfreeness, thereby retaining mean-field scaling by construction. Numerical investigations of dissociation processes in strongly correlated molecular systems show that this conjectured linearity holds for bond breaking dominated by paired bonding-antibonding orbitals, but breaks down for heterolytic dissociation and excited states. In regimes where the correlation conjecture is valid, i-DMFT yields indeed reasonable total energies but fails to reliably reproduce 1RDMs and individual energy components. These findings establish practical criteria for the applicability of i-DMFT and clarify the limitations of linear entropy-energy relations in 1RDM functional design.

Kinetic Energy Tensors: Importance of Anisotropy in Chemical Analysis

Gautam Jha

Understanding the bonding in chemical systems is one of the prime focus of quantum chemistry and most of the current analyzes are developed on the premise of density functional theory (DFT). DFT relies heavily on the exchange correlation (XC) functionals where the exchange energy is calculated from the Taylor expansion of a spherically averaged exchange hole which eliminates information about the anisotropy of the related properties of the exchange hole. The Taylor expansion expresses the exchange hole curvature in terms of kinetic energy density. Several formulations exist which connect the bonding scenarios to kinetic energy density, such as electron localization functions (ELF). Here, we have investigated bonding in chemical systems by taking the tensor forms of the kinetic energy density rather than the scaler form calculated by spherical averaging. This approach provides us with additional insights such as anisotropy of the bonding modes and opens the path for inclusion of exchange hole anisotropy in kinetic energy based Meta-GGA DFT functionals.

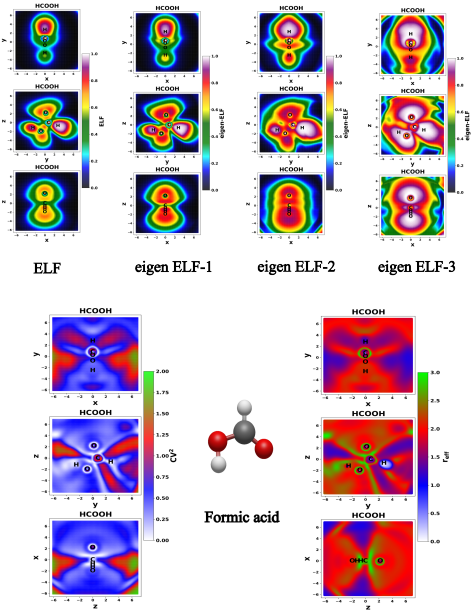

Figure 3.2: ELF, eigen-ELFs, and anisotropy plots of **Formic Acid** (**HCOOH**).ε $= \mathbf{1e-03}$, $\tau_{\mathbf{ref}} = \tau_{\mathbf{TF}}$

A Convex-Analytic Formulation of the Møller–Plesset Adiabatic Connection

Elias Polak

The Møller–Plesset Adiabatic Connection (MPAC) theory provides a rigorous framework connecting the Hartree-Fock (HF) reference system to the fully interacting electronic system through a λ-dependent Hamiltonian [1]. At $\lambda = 0$ this Hamiltonian reduces to the Fock operator, while $\lambda = 1$ recovers the true physical electronic Hamiltonian. In analogy to adiabatic connection density functional theory (DFT) [2], MPAC enables formally exact definitions of exchange and correlation contributions relative to an HF reference, thereby offering a promising pathway for the construction of systematically improvable electronic-structure models. However, existing quantum chemistry formulations of MPAC are usually provided only for non-degenerate HF solutions, leaving the degenerate case elusive. In this work, we propose a convex-analytic formulation of MPAC based on an integral representation derived from the concavity of the ground-state energy with respect to the coupling parameter $\lambda > 0$. The corresponding energy is expressed in terms of density matrices Γ^λ–a representation that holds equally well for both pure and mixed states, thus, allowing the consistent treatment of degeneracies. Using this formulation, we derive exchange and correlation functionals for general HF states and establish key adiabatic connection properties that parallel fundamental results in adiabatic connection DFT. Additionally, a virial relation [3,4] is given in this setting which admits exact constraints in terms of the potential and density only. Numerical examples illustrate the behavior of MPAC integrals for different λ-dependent energy functions and confirm the theoretical predictions derived from the convex-analytic framework.

[1] K. J. Daas, H. Zhao, E. Polak, and S. Vuckovic, *Exact Moller-Plessen adiabatic connection correlation energy densities*, J. Chem. Theory Comput. **21** (11), 5501 – 5513 (2025).

[2] E. Polak, K. J. Daas, and S. Vuckovic, *The adiabatic connection formalism in DFT – theory and practice*, Chem. Modell. **18**, Royal Society of Chemistry, 1-17 (2024).

[3] I. Theophilou, M. Penz, M. Ruggenthaler, and A. Rubio, *Virial relations for electrons coupled to quantum field models*, J. Chem. Theory Comput. **16**, 6236 - 6243 (2020).

[4] A. Laestadius *et. al.*, *Exchange-only virial relation from the adiabatic connection*, J. Chem. Phys. **160** (2024).

Mean-field theory of ultrafast laser-driven quantum dynamics in positronium chloride

Thomas Bondo Pedersen

When an electron comes into contact with its antiparticle, the positron, the pair decays into (typically) two gamma photons at 511 keV each. This quantum electrodynamical positron annihilation process is crucial for medical diagnostics through positron emission tomography and its recent extension to positronium imaging (PI). The PI technique exploits the formation of short-lived positronium (Ps) "atoms", the hydrogen-like state of a positron and an electron bound by their Coulomb interaction, inside the body. The key feature exploited for imaging is the strong dependence of the lifetime on the surroundings of Ps. Similarly, positron annihilation lifetime spectroscopy has evolved into an important characterization technique in chemistry and material science.

Despite the advanced medical and scientific applications of positron annihilation, the bound states formed by positrons and atoms or molecules have proven very challenging to study theoretically. This poses a problem for further development of positron-based technologies and for fundamental scientific investigations of, e.g., exotic positron-mediated chemical bonding. The main obstacle is the high-level many-body theory required to accurately describe electronic and electron-positron correlations and to predict positron affinities of atoms and molecules. Experimentally, molecular positron affinities can be measured indirectly through vibrational Feshbach resonances while alternative techniques have been proposed for atoms. However, with lifetimes on the order of nanoseconds, it should be possible to study positron–matter binding and dynamics directly by ultrafast spectroscopy.

In this talk, I will present a computational study of the laser-driven quantum dynamics of positronium (Ps), PsH, and PsCl at the time-dependent Hartree–Fock level of theory [1]. To eliminate finite-basis effects and to properly capture continuum dynamics, we use a spherical polar pseudospectral representation. It is found that while the presence of the positron delays electron ionization in PsH, a slight enhancement of electron ionization is observed in PsCl. In both cases, the positronic response is faster than that of the electrons. It is proposed that the formation of PsCl may be directly observed through photopositron spectra in the multiphoton regime, where PsCl peaks are expected at roughly twice the energy of Ps peaks, making PsCl clearly distuinguishable from Ps. In the tunelling regime, however, photopositron rescattering peaks may only be distuinguishable if the amount of Ps is sufficiently low.

Joint work with E. Aurbakken, H. E. Kristiansen, S. Kvaal, A. Camper.

[1] E. Aurbakken, H. E. Kristiansen, S. Kvaal, A. Camper, T. B. Pedersen, *Ultrafast laser-driven quantum dynamics in positronium chloride*, arXiv:2603.17203 (2026).

Rigorous foundations of density-functional theory for one-dimensional systems

Thiago Carvalho Corso

In this talk, we review some recent results aiming towards a rigorous formulation of density functional theory (DFT) for one-dimensional systems. More precisely, we first present a complete solution of the v-representability problem for electrons trapped in a 1D bounded domain (under suitable boundary conditions). In this setting, we then present a quantitative version of the Hohenberg–Kohn theorem for distributional potentials. Together, these results can be used to establish the existence of an exact exchange-correlation potential and to put the forward and inverse Kohn–Sham scheme on a rigorous mathematical ground. Furthermore, they allow us to establish the existence of the adiabatic connection potential and study its regularity with respect to the density and the interaction strength. Time permitting, we shall also highlight how these results can be used to justify the asymptotic expansion of the adiabatic potential in the weakly interacting limit, also known as the Görling–Levy perturbation series, and in the strongly interacting limit, also known as the strictly correlated regime. These results are based on the following references:

[1] T.C. Corso, *A rigorous formulation of density functional theory for spinless fermions in one dimension*. Lett Math Phys **116**, 27 (2026).

[2] T.C. Corso, *A Non-degeneracy Theorem for Interacting Fermions in One Dimension*. Ann. Henri Poincaré (2026).

[3] T.C. Corso and A. Laestadius, *A quantitative Hohenberg–Kohn theorem and the unexpected regularity of density functional theory in one spatial dimension*, arXiv:2512.04726 **[math-ph]** (2025).

[4] T.C. Corso, *Strictly correlated electrons in a quantum ring: from Kohn–Sham to Kantorovich potentials*, arXiv:2604.09908 **[math-ph]** (2026).

A novel mathematical framework for DFT and RDMFT

Håkon Fredheim

In this talk, I will present my recent work with Simen Kvaal ([arXiv:2510.12242] Reduced Density Matrix Functional Theory And A Reduced Formulation Of Density Functional Theory), where we introduce a novel mathematical framework for DFT and RDMFT. This framework involves a "natural" Banach space structure. I will present some further results in this framework.

1968: Solution to the Finite Size Effect within Mean-field Theories

Kangbo Li

The Born-von-Karman periodic boundary conditions (PBCs) has been a standard assumption in computational condense matter Physics and condense phase Chemistry. The PBCs are sometimes understood to be unphysical but nevertheless a natural combination with plane-wave infrastructures and the celebrated Bloch theorem. The caveat is that they truncate the particle number of an infinite system, causing the finite size effect. This error can be corrected in many ways, but the corrections obscure an otherwise elegant theory. In this talk, we show that within mean-field theories, the PBCs and thus the finite size effect can be analytically lifted by replacing Bloch-waves with k-space wave-packets as in semi-classical electron transport. In 1D, this formalism is a rediscovery of an early quantum theory of polymers by Jean Marie André, which was later bent into compliance with Bloch theorem, reintroducing the finite size effect.

Maxwell-regularized density-functional theory

Markus Penz

A framework for DFT is proposed that takes the electrostatic Poisson equation as its foundation. It is formulated on a natural Sobolev space for potentials and the dual space for densities, and also takes the energy of the external potential into account. This leads to a fully regularized theory that avoids the usual representability problems. Consequences and generalizations of the novel framework are discussed.

Neural network approximation of regularized density functionals

Mathias Oster

Density-functional theory is one of the most efficient and widely used computational methods of quantum mechanics, especially in fields such as solid state physics and quantum chemistry. From the theoretical perspective, its central object is the universal density functional which contains all intrinsic information about the quantum system in question. Once the external potential is provided, in principle one can obtain the exact ground-state energy via a simple minimization. However, the universal density functional is a very complicated mathematical object and almost always it is replaced with its approximate variants. So far, no "first principles", mathematically consistent and convergent approximation procedure has been devised that has general applicability. In this talk, we propose such a procedure by first applying Moreau–Yosida regularization to make the exact functionals continuous (even differentiable) and then approximate the regularized functional by a neural network. The resulting neural network preserves the positivity and convexity of the exact functionals. More importantly, it is differentiable, so it can be directly used in a Kohn–Sham calculation.

[1] M. A. Csirik, A. Laestadius, M. Oster, *Neural network approximation of regularized density functionals.* arXiv:2511.18512 **[physics.chem-ph]** (2025).

Friday April 24th

Algorithmic differentiation for plane-wave DFT

Niklas Frederik Schmitz

We present a differentiation framework for plane-wave density-functional theory (DFT) that combines forward-mode algorithmic differentiation (AD) with density-functional perturbation theory (DFPT) [1]. Derivatives of any DFT output with respect to any input parameter (geometry, density functional, pseudopotential) are obtained by implicit differentiation of the Kohn–Sham equations, realised as a custom AD rule invoking the DFPT response solver at a converged solution. We implement AD-DFPT in the Density-Functional ToolKit (DFTK), with applications ranging from propagating parameter uncertainties and a-posteriori discretisation error estimates to quantities of interest, to inverse problems such as learning exchange-correlation parameters. Ongoing work extends AD-DFPT to reverse-mode AD via adjoint methods, scaling self-consistent gradient-based DFT workflows to high-dimensional parameter optimisation.

[1] N. F. Schmitz, B. Ploumhans, and M. F. Herbst. *Algorithmic differentiation for plane-wave DFT: materials design, error control and learning model parameters.* npj Computational Materials **12**, 6 (2026).

Recent advances in pushing back system-size and accuracy limitations in DFT

Vikram Gavini

This talk will discuss our recent advances in addressing the system-size and accuracy limitations in DFT. In particular, the development of computational methods and numerical algorithms for conducting fast and accurate large-scale DFT calculations using adaptive finite-element discretization will be presented, which form the basis for the recently released DFT-FE open-source code. The computational efficiency, scalability and performance of DFT-FE will be presented, which demonstrates a significant outperformance of widely used plane-wave DFT codes. Some recent application studies that highlight the capabilities of DFT-FE will be presented. In addressing the accuracy challenge, our approach to accurately solving the inverse DFT problem will be presented, which has enabled the computation of exact exchange-correlation potentials for polyatomic systems. Ongoing efforts on using the exact exchange-correlation potentials and energies to improve the exchange-correlation functional description in DFT will be discussed.

A mathematical approach to coupled-cluster theory

Simen Kvaal

TBA

Electron densities for atoms and small molecules from wavefunction methods with a pseudospectral basis

Håkon Kristiansen

TBA

Why is ice so slippery?

Sigbjørn Løland Bore

The origin of ice's slipperiness has been a subject of intense debate for centuries. In this talk, I will present work, in collaboration with Sveinsson, on modeling ice friction from first principles. Our approach uses machine-learning interatomic potentials trained on quantum-mechanical data to provide an unbiased description of ice friction at the nanoscale. By combining these molecular dynamics simulations with a frictional heating model, we connect our findings to the macroscale coefficient of friction. Our findings highlight the importance of frictional heating as a cause of ice slipperiness.

List of Participants

Aouina, Ayoub	Ruhr-Universität Bochum
Bachmayr, Markus	RWTH Aachen University
Bakkestuen, Vebjørn	Oslo Metropolitan University
Bohle, Oliver	Hylleraas Centre, University of Oslo
Bore, Sigbjørn	Hylleraas Centre, University of Oslo
Burke, Kieron	University of California, Irvine
Cancès, Eric	Ecole des Ponts - Institut Polytechnique de Paris and Inria
Corso, Thiago Carvalho	University of Stuttgart
Cort-Barrada, Luis	International Centre for Theory of Quantum Technologies
Duez, Théo	CNRS and Inria Paris
Falmår, Vegard	Oslo Metropolitan University
Faulstich, Fabian	Rensselaer Polytechnic Institute
Fredheim, Håkon	Hylleraas Centre, University of Oslo / Sopra Steria
Gavini, Vikram	University of Michigan
Garrigue, Louis	CY Cergy Paris University
Giarrusso, Sara	Technical University of Eindhoven
van Gog, Jari	Sorbonne Université
Gould, Tim	Griffith University
Graf, Paul	Ludwig-Maximilians-Universität München
Helgaker, Trygve	Hylleraas Centre, University of Oslo
Herbst, Michael	École Polytechnique Fédérale de Lausanne
Jöns, Christian	MPI for the Structure and Dynamics of Matter
Jha, Gautam	Hylleraas Centre, University of Oslo
Kristiansen, Håkon	Hylleraas Centre, University of Oslo
Kumar, Dharamveer	Indian Institute of Technology Bombay
Kvaal, Simen	Hylleraas Centre, University of Oslo
Laestadius, Andre	Oslo Metropolitan University
Lauritsen, Asbjørn	CNRS & CEREMADE, Université Paris Dauphine
van Leeuwen, Robert	University of Jyväskylä
Levitt, Antoine	Université Paris Saclay
Lewin, Mathieu	CNRS & Université Paris-Dauphin
Li, Kangbo	Rensselaer Polytechnic Institute

Liebert, Julia	Princeton University
Lotfigolian, Maryam	Oslo Metropolitan University
Matassa, Marco	Oslo Metropolitan University
Mercuri, Carlo	University of Modena and Reggio Emilia
Nevalaita, Janne	University of Jyväskylä
Oldenburg, Jakob	CNRS & Université Paris Dauphine
Oster, Mathias	RWTH Aachen University
Pedersen, Thomas	Hylleraas Centre, University of Oslo
Penz, Markus	Ludwig-Maximilians-Universität München & Oslo Metropolitan University
Pittalis, Stefano	NRC, Institute of Nanoscience, Modena, Italy
Polak, Elias	University of Fribourg
Rumiz, Francesco	University of Trieste
Schilling, Christian	Ludwig-Maximilians-Universität München
Schmitz, Niklas	École Polytechnique Fédérale de Lausanne
Szepessy, Anders	Royal Institute of Technology
Tancogne-Dejean, Nicolas	Ruhr-Universität Bochum
Tellgren, Erik	Hylleraas Centre, University of Oslo
Toulouse, Julien	Sorbonne Université & CNRS
Wang, Chih-Chun	Ludwig-Maximilians-Universität München

Notes