FAIR Data management of theoretical spectroscopy and green's function methods

April 20 - 23, 2026
CECAM-HQ-EPFL, Lausanne, Switzerland

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1. Description

Data-driven methodologies are now central to materials science, but their impact depends critically on effective data sharing. FAIR data management and open science enable data reuse, verification, and systematic exploitation across the vast chemical space of materials. While these approaches have been highly successful for ground-state materials discovery based on Density Functional Theory (DFT), similar progress has not yet been achieved for more advanced simulation frameworks.

Theoretical spectroscopy and Green's function methods, such as GW, TDDFT, BSE, DMFT, and KKR, are essential for describing excited-state properties and electronic correlations, yet they pose major FAIR data challenges. These simulations are computationally intensive, generate complex datasets, and rely on heterogeneous software ecosystems. Despite recent database efforts, limited interoperability and incomplete workflow provenance continue to hinder reproducibility and reuse.

Within the FAIRmat initiative, the NOMAD platform now supports theoretical spectroscopy and Green's function simulations, hosting large numbers of GW, BSE, and DMFT workflows with full provenance. The objective of this workshop is to address the remaining interoperability challenge by defining common data structures and workflows, enabling consistent data exchange, reproducibility, and large-scale reuse. Achieving this goal requires close collaboration between method developers, materials scientists, data scientists, and data management experts.

2. Program

Day 1 - Monday April 20th 2026

FOUNDATIONS & KICK-OFF

- 12:00 to 13:00 - Registration
- 13:00 to 13:15 - Welcome & Introduction

Session 1 - FAIR DATA

- 13:15 to 14:00 - **Claudia Draxl**
  FAIR data infrastructure

- 14:00 to 14:30 - **Gian-Marco Rignanese**
  Bridging the materials data ecosystem: OPTIMADE and the era of AI-driven interoperability

- 14:30 to 15:15 - **Esma Boydas**
  Nomad-simulations: A data model for machine-actionable materials science

- 15:15 to 15:45 - Coffee break

Session 2 - Frontiers in ultrafast and time-resolved theories

- 15:45 to 16:30 - **Felipe Jornada**
  Tuning light with materials and materials with light

- 16:30 to 17:15 - **Daria Gorelova**
  Theoretical description of ultrafast x-ray imaging and spectroscopy of electron dynamics

- 17:15 to 17:45 - **Andrea Marini**
  From semi–classical swings to retardation: The electron–phonon problem as the devil in the box of many–body theory

Day 2 - Tuesday April 21st 2026

CORRELATED METHODS & SPECTROSCOPY STANDARDS

Session 1 - DMFT

- 09:00 to 09:45 - **Leonard Verhoff**
  DMFT for strongly correlated materials

- 09:45 to 10:15 - **Erik van Loon**
  Data management for dynamical mean-field theory based approaches

Session 2 - GW

- 10:15 to 10:45 - **Mauricio Rodríguez-Mayorga**
  Open questions to making scGW a FAIR method

- 10:45 to 11:15 - Coffee break

- 11:15 to 12:00 - **Rémi Pasquier**
  Efficient GW band structure calculations using Gaussian basis functions and application to atomically thin transition-metal dichalcogenides

Session 3 – Electron-phonon coupling

- 12:00 to 12:45 - **Samuel Poncé**
  Data management for ARPES, superconductivity and transport. Importance of verification & validation

- 12:45 to 13:45 - Lunch

Session 4 - Multiple scattering, KKR spectroscopy, etc.

- 13:45 to 14:30 - **Jan Minár**
  Multiple scattering green function KKR method for electron spectroscopies

- 14:30 to 15:15 - **John Rehr**
  FAIR representation of real-space green's function spectroscopy calculations

- 15:15 to 15:45 - Coffee break

Session 4 – Roundtable: Core data objects for ultrafast spectroscopy

- 15:45 to 16:15 - **Luca Ghiringhelli**
  Introduction to data modeling and interoperability in practice

- 16:15 to 18:00 - **Luca Ghiringhelli** (moderator)
  Core data objects for ultrafast spectroscopy

- 19:00 to 22:30 - Social dinner

Day 3 - Wednesday April 22nd 2026

DATA MANAGEMENT: FILE FORMATS, SCHEMAS, & PARSERS

Session 1 – Code-specific data management

- 09:00 to 09:45 - **Maurits W. Haverkort**
  Embedded multi-reference many-body calculations for spectroscopy as implemented in quanty from a numerical data science perspective

- 09:45 to 10:30 - **Anna Hehn**
  Modeling excited states in solids: An attempt at a FAIR comparison of software packages

- 10:30 to 11:00 - Coffee break

- 11:00 to 11:15 - **Gian-Marco Rignanese**
  Data management in ABINIT through atomate2 workflows

- 11:15 to 11:30 - **Martin Kuban**
  The exciting code for theoretical spectroscopy

- 11:30 to 11:45 - **Alexey Tal**
  Data Management in VASP

- 11:45 to 12:00 - **Andrea Marini**
  Yambo 6: Dynamical modules and a new logical infrastructure

Session 2 – Schema & parser development

- 12:00 to 12:30 - **Elena Molteni**
  Implementing FAIR data management in the NFFA-DI distributed research infrastructure for nanoscience: The case of NOMAD parsers extensions for theory & simulation at the UMIL unit

- 12:30 to 13:30 - Lunch

- 13:30 to 14:15 - **Jose M. Pizarro, Esma Boydas**
  Schema studio demo

- 14:15 to 15:15 - **Patrick Rinke, Joseph Rudzinski** (Moderators)
  Hands-on Session: Schema development for methods and workflows

- 15:15 to 15:45 - Coffee break

- 15:45 to 17:15 - **Patrick Rinke, Joseph Rudzinski** (Moderators)
  Hands-on Session: Schema development for methods and workflows

- 17:15 to 19:00 - Poster session & aperitif

Day 4 - Thursday April 23rd 2026

DATA SCIENCE, WRAP-UP, & HANDS-ON

Session 1 - AI/ML/Workflow

- 09:00 to 09:45 - **Jan Janssen**
  FAIR data management with the pyiron workflow framework

- 09:45 to 10:30 - **Martin Kuban**
  Measuring convergence with spectral fingerprints

- 10:30 to 11:00 - Coffee break

Session 2 - Wrap-up

- 11:00 to 12:00 - **Luca Ghiringhelli** (moderator)
  Roundtable: Synthesis of findings, Community roadmap, Data policy alignment, Funding and support, etc.

- 12:00 to 13:00 - Lunch

Session 3 - Hands-on Data Management

- 13:00 to 15:30 - **Joseph Rudzinski**
  NOMAD Tutorial (with short coffee break)

3. Abstracts

Core data objects for ultrafast spectroscopy

Luca Ghiringhelli (moderator)
Karlsruhe Institute of Technology (KIT), Germany

TBA

Bridging the materials data ecosystem: OPTIMADE and the era of AI-driven interoperability

Gian-Marco Rignanese
Université catholique de Louvain, Belgium

The last few decades have seen a proliferation of online materials databases. While these repositories offer powerful graphical web interfaces for manual, "low-throughput" exploration, they often lack the infrastructure required for systematic, high-throughput computational workflows. To fully leverage modern data analytics, these databases must expose robust Application Programming Interfaces (APIs). Furthermore, to harness the synergy between diverse material families and properties, a standardized query language is essential.

The **Open Databases Integration for Materials Design (OPTIMADE)** API was developed to solve these interoperability challenges [1,2]. Now supported by leading repositories–including AFLOW, Alexandria, Materials Cloud, Materials Project, NOMAD, and OQMD–OPTIMADE provides a unified specification for cross-database discovery.

In this talk, I will outline the core features of the OPTIMADE API and demonstrate its utility through practical examples. Additionally, I will introduce our current work on developing a **Model Context Protocol (MCP) for OPTIMADE**. This integration aims to bridge the gap between structured materials data and Large Language Models (LLMs), enabling AI agents to autonomously query and reason across the global materials science data landscape.

*[1] C. Andersen, R. Armiento, E. Blokhin, G. Conduit, S. Dwaraknath, M. Evans, Á. Fekete, A. Gopakumar, S. Gražulis, A. Merkys, F. Mohamed, C. Oses, G. Pizzi, G. Rignanese, M. Scheidgen, L. Talirz, C. Toher, D. Winston, R. Aversa, K. Choudhary, P. Colinet, S. Curtarolo, D. Di Stefano, C. Draxl, S. Er, M. Esters, M. Fornari, M. Giantomassi, M. Govoni, G. Hautier, V. Hegde, M. Horton, P. Huck, G. Huhs, J. Hummelshøj, A. Kariryaa, B. Kozinsky, S. Kumbhar, M. Liu, N. Marzari, A. Morris, A. Mostofi, K. Persson, G. Petretto, T. Purcell, F. Ricci, F. Rose, M. Scheffler, D. Speckhard, M. Uhrin, A. Vaitkus, P. Villars, D. Waroquiers, C. Wolverton, M. Wu, X. Yang, Sci. Data., **8**, 217 (2021)*

*[2] M. Evans, J. Bergsma, A. Merkys, C. Andersen, O. Andersson, D. Beltrán, E. Blokhin, T. Boland, R. Castañeda Balderas, K. Choudhary, A. Díaz Díaz, R. Domínguez García, H. Eckert, K. Eimre, M. Fuentes Montero, A. Krajewski, J. Mortensen, J. Nápoles Duarte, J. Pietryga, J. Qi, F. Trejo Carrillo, A. Vaitkus, J. Yu, A. Zettel, P. de Castro, J. Carlsson, T. Cerqueira, S. Divilov, H. Hajiyani, F. Hanke, K. Jose, C. Oses, J. Riebesell, J. Schmidt, D. Winston, C. Xie, X. Yang, S. Bonella, S. Botti, S. Curtarolo, C. Draxl, L. Fuentes Cobas, A. Hospital, Z. Liu, M. Marques, N. Marzari, A. Morris, S. Ong, M. Orozco, K. Persson, K. Thygesen, C. Wolverton, M. Scheidgen, C. Toher, G. Conduit, G. Pizzi, S. Gražulis, G. Rignanese, R. Armiento, Digital Discovery, **3**, 1509 (2024)*

Data management for ARPES, superconductivity and transport. Importance of verification & validation

Samuel Poncé
Université catholique de Louvain, Belgium

TBA

Data management for dynamical mean-field theory based approaches

Erik van Loon
Lund University, Sweden

Dynamical mean-field theory and its extensions are among the standard computational approaches for strongly correlated materials. They provide access to both single-particle Green's functions and dynamic susceptibilities. FAIR data management for DMFT-based approaches introduces some unique challenges: (1) Quantum Monte Carlo is often used as an impurity solver, which leads to intrinsically stochastic data. (2) To go from data obtained on the Matsubara axis to spectroscopy, it is necessary to perform analytical continuation, which introduces another form of uncertainty. How to best store and share this kind of data, and communicate its uncertainty? How much (actual, useful) information does a DMFT calculation contain? In this contribution, I will discuss recent work on these questions.

Data management in ABINIT through atomate2 workflows

Gian-Marco Rignanese
Université catholique de Louvain, Belgium

In this talk, I will discuss the strategies and infrastructure required for effective data management within the ABINIT ecosystem [1]. A central focus will be the integration of ABINIT with **atomate2**, a library of pre-defined, "best-practice" workflows [2]. By leveraging the **Jobflow-remote** workflow manager and the **Jobflow** library [3], atomate2 enables the orchestration of multi-step ABINIT tasks – such as structural relaxations followed by GW or DMFT calculations – with built-in error handling and automated data provenance.
I will demonstrate how these automated workflows streamline the path from raw input to database-ready output, ensuring that data is **FAIR** (Findable, Accessible, Interoperable, and Reusable). Finally, I will showcase how this structured approach to data management facilitates the high-throughput generation of materials descriptors, directly feeding into the broader OPTIMADE ecosystem.

[1] M. Verstraete, J. Abreu, G. Allemand, B. Amadon, G. Antonius, M. Azizi, L. Baguet, C. Barat, L. Bastogne, R. Béjaud, J. Beuken, J. Bieder, A. Blanchet, F. Bottin, J. Bouchet, J. Bouquiaux, E. Bousquet, J. Boust, F. Brieuc, V. Brousseau-Couture, N. Brouwer, F. Bruneval, A. Castellano, E. Castiel, J. Charraud, J. Clérouin, M. Côté, C. Duval, A. Gallo, F. Gendron, G. Geneste, P. Ghosez, M. Giantomassi, O. Gingras, F. Gómez-Ortiz, X. Gonze, F. Goudreault, A. Grüneis, R. Gupta, B. Guster, D. Hamann, X. He, O. Hellman, N. Holzwarth, F. Jollet, P. Kestener, I. Lygatsika, O. Nadeau, L. MacEnulty, E. Marazzi, M. Mignolet, D. O'Regan, R. Outerovitch, C. Paillard, G. Petretto, S. Poncé, F. Ricci, G. Rignanese, M. Rodriguez-Mayorga, A. Romero, S. Rostami, M. Royo, M. Sarraute, A. Sasani, F. Soubiran, M. Stengel, C. Tantardini, M. Torrent, V. Trinquet, V. Vasilchenko,

D. Waroquiers, A. Zabalo, A. Zadoks, H. Zhang, J. Zwanziger, The Journal of Chemical Physics, ***163****, 164126 (2025)*

[2] A. Ganose, H. Sahasrabuddhe, M. Asta, K. Beck, T. Biswas, A. Bonkowski, J. Bustamante, X. Chen, Y. Chiang, D. Chrzan, J. Clary, O. Cohen, C. Ertural, M. Gallant, J. George, S. Gerits, R. Goodall, R. Guha, G. Hautier, M. Horton, T. Inizan, A. Kaplan, R. Kingsbury, M. Kuner, B. Li, X. Linn, M. McDermott, R. Mohanakrishnan, A. Naik, J. Neaton, S. Parmar, K. Persson, G. Petretto, T. Purcell, F. Ricci, B. Rich, J. Riebesell, G. Rignanese, A. Rosen, M. Scheffler, J. Schmidt, J. Shen, A. Sobolev, R. Sundararaman, C. Tezak, V. Trinquet, J. Varley, D. Vigil-Fowler, D. Wang, D. Waroquiers, M. Wen, H. Yang, H. Zheng, J. Zheng, Z. Zhu, A. Jain, Digital Discovery, ***4****, 1944 (2025)*

[3] A. Rosen, M. Gallant, J. George, J. Riebesell, H. Sahasrabuddhe, J. Shen, M. Wen, M. Evans, G. Petretto, D. Waroquiers, G. Rignanese, K. Persson, A. Jain, A. Ganose, JOSS., ***9****, 5995 (2024)*

Data management in VASP

Alexey Tal
VASP Software GmbH, Austria

TBA

DMFT for strongly correlated materials

Leonard Verhoff, Karsten Held, Liang Si
TU Wien, Austria

TBA

Efficient GW band structure calculations using Gaussian basis functions and application to atomically thin transition-metal dichalcogenides

Rémi PASQUIER[1], María Camarasa-Gómez[2], Anna-Sophia Hehn[3], Daniel Hernangómez-Pérez[4], Jan Wilhelm[1]
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[2]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Spain
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The *GW* approximation is widely used to compute self-energies and related electronic properties but remains computationally demanding, motivating the development of more efficient approaches. We present a space-time *GW* algorithm for periodic systems in a Gaussian basis with spin-orbit coupling, enabling accurate and efficient quasiparticle band-structure calculations for atomically thin materials. For monolayer MoS_2, $MoSe_2$, WS_2, and WSe_2, the resulting *GW* band gaps agree on average within 50 meV with plane-wave reference values. Full G_0W_0 band structures can be computed in less than two days on a laptop (Intel i5, 192 GB RAM) or under 30 minutes using 1024 cores.

[1] R. Pasquier, M. Camarasa-Gómez, A. Hehn, D. Hernangómez-Pérez, J. Wilhelm, Phys. Rev. B, ***112****, 205130 (2025)*

Embedded multi-reference many-body calculations for spectroscopy as implemented in quanty from a numerical data science perspective

Maurits W. Haverkort
University of Heidelberg, Germany

TBA

FAIR data infrastructure

Claudia Draxl
Humboldt-Universität zu Berlin, Germany

TBA

FAIR data management with the pyiron workflow framework

Jan Janssen
Max Planck Institute for Sustainable Materials, Germany

TBA

FAIR representation of real-space green's function spectroscopy calculations

John Rehr[1], J.J. Kas[1], F.D Vila[1], A. Kaplan[2], P. Huck[2], T. Mathis[2]
[1]University of Washington, United States
[2]Lawrence Berkeley National Laboratory, United States

The real-space Green's function (RSGF) approach, aka real-space KKR, as implemented in the FEFF codes has been widely used for theoretical spectroscopy calculations. They include x-ray absorption (XAS), emission (XES), electron energy loss spectra (EELS) and others. Due to their computational efficiency, FEFF is well suited for compiling training sets for ML applications. In an effort to enhance their utility for data-driven applications, we have created a trial input/output structure for FEFF calculations of XAS consistent with FAIR data management principles. This structure uses a standardized JSON input/output format that includes meta-data needed to characterize and replicate a given spectral calculation. This type of representation is also necessary to bring FEFF XAS calculations into FAIR compliance, and keep parity with existing FAIR-compliant Materials Project (MP) XAS data. Likewise, it is desirable to develop a standardized input/output structure for calculations of similar spectra with other codes. They include Bethe-Salpeter-Equation calculations using OCEAN, exciting!, and related quantum-chemistry codes like NWChem. Extensions of the format to Corvus workflows that combine auxiliary codes for more complex calculations are also desirable. Such extensions would enable FAIR representations of optical constant calculations for all materials in the MP data base.

From semi-classical swings to retardation: The electron-phonon problem as the devil in the box of many-body theory

Andrea Marini
CNR, Italy

Electrons and phonons are basic concepts, considered as the most elemental and well defined example of fermions and bosons. So it may appear that their formal properties are clear and well established. In reality, despite books and reviews the theory of electron-phonon interaction(EPI) is still very much debated. The reason is mostly historical. Indeed the state-of-the art theoretical and numerical approach to the EPI has been built on top of two popular methods: model Hamiltonians and Density Functional Perturbation Theory (DFPT). These popular approaches have instilled two basic assumptions that are widely used in the literature and even coded in public Ab–Initio codes.

The first assumption is that the elemental EPI Hamiltonian is well approximated by using a statically screened interaction.

The second assumption is clearly written in a recent Review of Modern Physics of F. Giustino where he writes that “the MBPT phonon self-energy is in agreement with the expression derived starting from time-dependent density-functional perturbation theory”.

In this talk I will disassemble the EPI Hamiltonian to demonstrate its stringent limitations. I will also introduce a time-dependent formulation of DFPT showing how it can be exactly rewritten as the problem of a classical pendulum immersed in a quantistic liquid (semi-classical swing). I will discuss the countless implications of such a problem linked the very basic foundations of MBPT.

I will then move to present a formal an accurate derivation 3 of the dynamical screening of the EPI. I will, in particular, demonstrate that it is possible to derive an effective vertex correction function that can be easily defined using simple ingredients and used to amend calculations based on the statically screened approximation.

*[1] A. Marini, Phys. Rev. B, **110**, 024306 (2024)*
[2] Marini, A. Dynamical electron-phonon vertex correction, arXiv:2501.01866 (2025)

Implementing FAIR data management in the NFFA-DI distributed research infrastructure for nanoscience: the case of NOMAD parsers extensions for theory & simulation at the UMIL unit

Elena Molteni
Università degli Studi di Milano, Italy

The NFFA-DI project (Nano Foundries and Fine Analysis - Digital Infrastructure, nffa-di.it) aims at building an italian distributed Research Infrastructure (RI) for nanoscience and nanotechnology. It envisages access by external users to multiple facilities of the distributed RI – ranging from materials growth to several experimental materials characterization techniques and to computational methods - through a Single Entry Point (SEP) and regular calls for proposals, and it has a focus on the FAIR-by-design management of research data.

The NFFA-DI project has chosen NOMAD as Data Repository for the upload, storage and publishing of its research data in a structured way according to the FAIR principles, by setting up a project Oasis on its OFED (Overarching FAIR Ecosystem for Data) data repository; all the NFFA-DI Operative Units (OU) are setting up their FAIR-by-design pipelines so to produce research data in NOMAD-compatible formats.
After presenting the NFFA-DI project, its aims and the results achieved so far, I will discuss the work we are performing in the Theory&Simulation part of the UMIL (Università degli Studi di Milano) Operative Unit of NFFA-DI. The simulation codes our group is offering through the NFFA-DI SEP and "Catalogue" (QuantumEspresso, Yambo, Siesta, LAMMPS) are already NOMAD-supported. However, we have identified several possible extension opportunities in the NOMAD parsers for the mentioned codes, in order to widen the range of data and metadata NOMAD can extract from their input and output files, and we have started working on some of them in close collaboration with the FAIRmat team.
In particular I will focus on our ongoing work on two extensions of the NOMAD Yambo parser, aimed at:
1) the correct parsing of atom coordinates and number of atoms by chemical species
2) the parsing (and plotting) of optical spectra.

Introduction to data modeling and interoperability in practice

Luca Ghiringhelli
Karlsruhe Institute of Technology (KIT), Germany

Following the introduction to the FAIRmat Data Infrastructure by Claudia Draxl, I will introduce some basic concepts about the modeling of materials-science data and sketch a roadmap towards achievement of interoperability (the "i" in FAIR) in the data storage and stewardship. This will be put in the wider context of the Repeatability and Replicability of computational and experimental materials science data.

Measuring convergence with spectral fingerprints

Martin Kuban
Humboldt Universität zu Berlin, Germany

TBA

Modeling excited states in solids: An attempt at a fair comparison of software packages

Anna Hehn
Christian-Albrechts-University Kiel, Germany

Motivated by the aim of describing the plethora of photochemical processes in solids, the current status for the quantum-mechanical tool set within the electronic-structure code CP2K and the mixed quantum classical dynamics code Newton-X will be presented, with recent developments ranging from surface hopping dynamics over perturbative spin-orbit coupling to the inclusion of static or dynamic correlation. Furthermore, data management within CP2K-NewtonX as well as the comparison with program packages for molecular quantum chemistry will be discussed based on the Gaussian and augmented plane wave ansatz.

*[1] J. Vogt, M. Schulz, R. Souza Mattos, M. Barbatti, M. Persico, G. Granucci, J. Hutter, A. Hehn, J. Chem. Theory Comput., **21**, 10474 (2025)*

Multiple scattering green function KKR method for electron spectroscopies

Jan Minar
University of West Bohemia, Czech Republic

TBA

NERxiv: A named entity recognition approach for structured metadata extraction from arXiv papers

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We present NERxiv, an open-source Python package for extracting structured metadata from arXiv papers, focusing on Strongly Correlated Electron Systems. Combining automated fetching, semantic chunking, and LLM-based reasoning, NERxiv enables systematic identification of computational methods (such as Dynamical Mean-Field Theory) metadata supporting reproducibility, benchmarking, and large-scale analysis.

Nomad-simulations: A data model for machine-actionable materials science

Esma Birsen Boydas
Humboldt-Universität zu Berlin, Germany

TBA

Open questions to making scGW a FAIR method

Mauricio Rodríguez-Mayorga, P-F Loos
Laboratoire de Physique Théorique, France

As of today, the knowledge on how to perform G0W0 or quasi-particle self-consistent GW (qsGW) calculations is well known among the condensed matter physics and chemistry communities. It is well accepted that efficient implementations should exploit density fitting techniques and use imaginary times and frequencies grids (including accurate weights to perform Fourier transforms among these representations). Thanks to the normalization of the GW procedure, condensed matter physicists and computational chemists have implemented this scheme and extended the applicability of Green's function-based methods to study extended systems and molecules,which makes these methods nowadays a routine in numerical simulations. Currently, this normalized scheme is available in many codes (e.g., SCM-ADF, ABINIT, FHI-aims, CP2K, etc.). Interestingly, to further improve the normalization of these methods, the greenX library was recently released,

which will certainly extend the number of computational software packages incorporating efficient Green's functions-based methods. However, moving towards fully self-consistent GW schemes (scGW) still presents many open questions that need to be addressed and normalized before their applicability can be extended in the community (e.g., the non-conservation of the number of electrons during the self-consistent procedure). In this contribution, I will present the open questions that should be addressed, as well as possible solutions that should contribute to making scGW calculations a more FAIR method to the community.

The exciting code for theoretical spectroscopy

Martin Kuban
Humboldt Universität zu Berlin, Germany

TBA

Theoretical description of ultrafast x-ray imaging and spectroscopy of electron dynamics

Daria Gorelova
Brandenburg University of Technology Cottbus Senftenberg, Germany

In my talk, I will focus on projects that rely specifically on the post-processing of ab initio calculations performed by external codes.
The first project is the development of an ab initio scheme based on the Bethe-Salpeter equation (BSE) for the description of optical pump–resonant x-ray probe techniques [1, 2]. It treats both valence-excited and core-excited states at the same level of theory using the output of the BSE calculations with the full-potential linearized augmented-plane-wave method implemented in the *exciting* package.
Other projects are about ultrafast x-ray probes of materials during the time they are dressed by optical light. I will present our ab initio description of x-ray diffraction and absorption spectroscopy of materials while they are optically driven by light. Our schemes rely on computing laser-dressed states using the Floquet-Bloch formalism [3,4], and analyzing x-ray-induced transitions within laser-dressed states [5,6]. We calculate x-ray diffraction of laser-dressed materials using the output of the ABINIT package. X-ray absorption of laser-dressed materials is calculated using the output of the *exciting* package.

*[1] N. Farahani, D. Popova-Gorelova, Phys. Rev. B, **110**, 235126 (2024)*
[2] Martí Raya-Moreno et al., An exciting approach to theoretical spectroscopy, arXiv:2601.11388 (2026)
*[3] D. Popova-Gorelova, R. Santra, Structural Dynamics, **11**, 014102 (2024)*
[4] Tatiana Bezriadina and Daria Popova-Gorelova, Laser-dressed partial density of states, arXiv:2505.19894 (2025)
[5] Chance Ornelas-Skarin, Tatiana Bezriadina, Matthias Fuchs, Shambhu Ghimire, J. B. Hastings, Quynh L Nguyen, Gilberto de la Peña, Takahiro Sato, Sharon Shwartz, Mariano Trigo, Diling Zhu, Daria Popova-Gorelova, and David A. Reis, Second-order microscopic nonlinear susceptibility in a centrosymmetric material: Application to imaging valence electron motion, Phys. Rev. X 16, 011006 (2026)
*[6] D. Popova-Gorelova, D. Reis, R. Santra, Phys. Rev. B, **98**, 224302 (2018)*

Tuning light with materials and materials with light

Felipe Jornada
Stanford University, United States

Optical responses have long served as powerful fingerprints for characterizing materials, with recent efforts in monolayer systems – featuring coupled valley and spin excitations, strongly bound excitons, and multiparticle complexes – as contemporary examples. This talk explores how to not only understand but also *actively modify* excited-state properties in materials using ultrafast and nonequilibrium drives, enabled by advances in parameter-free calculations based on many-body perturbation theory.
We will discuss nonlinearities predicted in the optical properties of monolayer materials and show how to understand them in terms of an exciton-driven Bloch–Floquet effect. We will also showcase recent method developments that give us access to optically induced structural changes in materials. In particular, we show how to compute unique fingerprints associated with optically excited materials, such as their vibrational spectra, which can be uniquely useful in problems ranging from photocatalysis to strongly driven matter.

Ultrafast nonlinear optics in solids: Analytical response models and the path to GW-BSE simulations with Gaussian orbitals

Jan Wilhelm
University of Regensburg, Germany

TBA

4. Posters

A DFT study on the role of excitons and electric field-induced symmetry breaking and topological properties of ZrBr

Halima Zaari
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The control of band gap and topological properties is a crucial objective in the field of materials science, particularly for the application of 2D materials such as topological insulators. Zirconium monobromide (ZrBr), a topological insulator with band inversion, holds significant potential for various applications. In this study, we used Density Functional Theory (DFT) with different approximations namely, Generalized Gradient Approximation (GGA) with and without spin orbit coupling (SOC) as well as hybrid functional to investigate the electronic structure and the band gap of this compound. In addition, we introduced the excitonic effect by considering GW plus Bethe–Salpeter equation (GW-BSE) to compute the optical band gap and quasi-particle energy. We found that ZrBr present a low static dielectric function and weak exciton binding energy, generally lower than those of conventional semiconductors. This behavior is due to the reduced Coulomb interaction in the material. To further explore the material's behavior, we apply an electric field in three directions to observe symmetry breaking and its impact on band gap tuning. This comprehensive analysis aims to explore the understanding and the potential applications of ZrBr as a topological insulator.

ATLAS-SPRKKR: A FAIR high-throughput ab initio database for machine learning in ARPES

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We present ATLAS-SPRKKR, a FAIR-compliant computational database built as a subpackage of ASE2SPRKKR, designed to support machine learning applications in angle-resolved photoemission spectroscopy. The database is populated through high-throughput SPR-KKR one-step photoemission calculations automated by the SparkkFlow workflow engine, which handles job scheduling, monitoring, and structured data collection across HPC environments at scale.

Each entry stores the complete calculation output in a self-describing HDF5 schema: converged full-potential relativistic Kohn-Sham data, layered-KKR slab geometry, FPA shape functions, photon and polarisation parameters including the full Stokes vector and Jones vector, and the four-channel ARPES cross-section I(k∥,E)I(k_\parallel, E) I(k∥,E) with provenance metadata compatible with NOMAD/FAIRmat. A Python client provides structured queries and auto-generates a 128-dimensional ML feature vector per entry encoding spectral, dichroic, spin-texture, and structural descriptors.

As a demonstration, the database was used to train a neural network for AI-assisted beam polarisation calibration in ARPES, using graphene as a symmetry-constrained calibration standard. The model achieves near-100% polarisation precision and enables real-time adaptive beamline control — the first integration of ab initio photoemission theory into experimental feedback loops.

This work establishes a reusable, open infrastructure connecting first-principles simulation, FAIR data curation, and data-driven spectroscopy.

Bandgap engineering in functionalised 2H-MoS2 with ab initio methods

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Monolayer 2H-MoS2 is a direct-gap semiconductor and acts as a promising candidate for photoexcitation and optoelectronic devices. Molecular functionalisation offers a promising route for bandgap engineering in two-dimensional materials, in general, enabling controlled tuning of their electronic and optical properties. In this study, we employ first-principles calculations to investigate charge-transfer processes in 2H-MoS2 under a two-sided Janus functionalisation scheme incorporating suitable donor-acceptor pairs. Additionally, we explore the impact of coverage-dependent effects, where the interaction of MoS2 with varying concentrations of differently fluorinated tetracyanoquinodimethane derivatives is systematically analysed. Besides these physisorbed molecules, we also investigate covalently bound systems on MoS2, such as methyl, trifluoromethyl, and phenyl derivatives. In this work, both the reaction mechanism for covalent functionalisation and the resulting changes in the electronic properties of the MoS2 layer are analysed. To further enhance the accuracy in the evaluation of electronic properties, screened hybrid functionals such as HSE06 and many-body perturbation theory within the GW approximation are employed, with the latter explicitly accounting for quasiparticle corrections. This is then combined with a BSE approach to account for electron-hole interactions and provide insight into the optical properties of the system.

*[1] S. Ray, B. Paulus, Nanomaterials, **15**, 193 (2025)*

Climbing Jacob's ladder for the coulomb hole

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Semilocal density functionals such as PBE typically underestimate experimental band gaps by 50%. Hybrid functionals address this "band gap problem" by admixing a fraction of Fock exchange to semi-local exchange. The optimal mixing parameter depends on the specific material and can be identified as the inverse dielectric constant [1]. Recently, we have shown that dielectric constants obtained using the r²SCAN meta-GGA functional [2] are significantly more accurate than dielectric constants obtained using PBE [3]. Furthermore, a dielectric-dependent hybrid functional based on r²SCAN can outperform the standard PBE-based hybrid in terms of band gaps [3]. Here, we showcase how the approximation for the DFT base functional relates to generalized Kohn-Sham and *GW* theories. Furthermore, we will present recent applications to challenging materials, including narrow-gap semiconductors and strongly correlated transition metal oxides.

*[1] A. Alkauskas, P. Broqvist, A. Pasquarello, Physica. Status. Solidi. (b)., **248**, 775 (2011)*
*[2] J. Furness, A. Kaplan, J. Ning, J. Perdew, J. Sun, J. Phys. Chem. Lett., **11**, 8208 (2020)*
[3] S. Riemelmoser, X. Xu and A. Pasquarello, Climbing Jacob's Ladder for the Coulomb hole: Dielectric-dependent hybrid functional based on meta-GGA, submitted to Nature Communications

Combining high-throughput computation and experimentation for AI-assisted inverse design of lead-free double perovskites for photovoltaics

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RT-BSE for optical properties of molecules

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Strain-tunable electronic and lattice thermal properties of Fe3GaTe2

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