O 38: Poster: Electronic Structure Theory

Time: Tuesday 18:00–20:00 Location: Poster D

O 38.1 Tue 18:00 Poster D

Pythonizing VASP: unleashing the power of collaboration in electronic structure theory — •Martin Schlipf[1], Sudarshan Vijay[1], and Georg Kresse[1,2] — [1]VASP Software GmbH, Berggasse 21, 1090 Vienna, Austria — [2]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, 1090 Vienna, Austria

The Vienna Ab-initio Simulation Package (VASP) provides powerful capabilities for materials simulations. In this presentation, we describe our new interface between VASP and the Python ecosystem that enhances data handling and empowers users to tailor VASP's behavior through Python scripting.

Currently, the diverse tools for VASP require text-based parsing of the output of the calculations. To avoid future Python packages reimplementing this fragile parsing, we introduce a structured output in HDF5 format and implement a parsing tool—*py4vasp*. With py4vasp, we obtain the data in Python dictionaries and provide postprocessing functionality like plotting and visualization.

In addition, we recognize the desire of many users to modify VASP's behavior. We discuss a novel interface that executes Python code from within a VASP calculation. By providing this entry point, users can change, for example, the potential, the energies, or the forces and extend VASP functionalities according to their specific research needs.

O 38.2 Tue 18:00 Poster D

Accelerating plane-wave-based *ab initio* molecular dynamics by optimization of Fast-Fourier transforms for modern HPC architectures — •Christian Ritterhoff, Tobias Klöffel, Sagarmoy Mandal, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

The most important advantage of plane-wave basis sets is that wave functions can be transformed efficiently from reciprocal to real space and back by using the Fast-Fourier transform (FFT) algorithm. This allows to evaluate the kinetic and potential energy in reciprocal and real space, respectively, where both operators are diagonal. This reduces the computational cost for applying the Hamilton operator from N^2 to $N \log N$. However, the scalability of current FFT libraries is rather limited on today's HPC systems, which offer large numbers of compute nodes, each of them with many cores. Here we present our optimization of the FFT routines in the Car-Parrinello molecular dynamics code CPMD (www.cpmd.org). Data distribution and communication patterns have been revised to make optimal use of combined MPI and OpenMP parallelization. Scalability is further increased by combining FFTs into batches and by introducing overlapping computation and communication. The improved performance of the new FFT routines will be demonstrated by a series of benchmark simulations with our optimized version of the CPMD code [1].

[1] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745

O 38.3 Tue 18:00 Poster D

Simulation of time-resolved RIXS spectra of laser-excited La2CuO4 based on multiplet ligand-field theory using Wannier orbitals — •Nils Brouwer[1], Maurits W. Haverkort[2], Sina Shokri[2], and Alexander I. Lichtenstein[1,3] — [1]European X-Ray Free-Electron Laser Facility, Holzkoppel 4, 22869 Schenefeld, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [3]Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany

Recent advancements in X-ray free electron laser science allow for the measurement of resonant inelastic X-ray scattering (RIXS) spectra of optically excited materials on the femtosecond time scale. Naturally, these advancements pose increasing challenges for theory to follow up with reasonable accuracy. This is especially true for highly correlated materials like La2CuO4, which often display very interesting functional properties.

In this work, following the method presented in reference [1], we apply multiplet ligand-field theory on a single site copper cluster and a multi-site copper cluster. Both clusters are parametrized by all electron DFT calculations of La2CuO4 using Wannier orbitals. Then, we calculate the time evolution of the laser-excited state of the cluster using the Krylov basis. Finally, we present RIXS spectra based on the time evolution of the laser-excited state.

[1]Phys. Rev. B 85, 165113 (2012)