

Automated High-Throughput Workflows for the All-Electron Full-Potential code exciting

Author: Fabian Peschel

Co-author: Claudia Draxl

Advances in computational materials science are increasingly driven by automated, reproducible, and scalable workflows that enable high-throughput exploration of materials properties. While such approaches have become well established for pseudopotential-based methods, equivalent frameworks for all-electron calculations remain comparatively scarce despite their importance for predictive simulations and computational accuracy.

We present `excitingworkflow`, a Python-based workflow framework for the all-electron full-potential code `exciting`. Built on the jobflow ecosystem, the framework provides modular and extensible workflows that automate complex simulation protocols, support robust execution on HPC systems, and enable systematic high-throughput studies with minimal user intervention. The framework incorporates automatic error handling, restart capabilities, provenance tracking, and flexible execution on local and remote computing resources.

The capabilities of `excitingworkflow` are demonstrated through several applications. First, we present a high-throughput equation-of-state workflow for calculating equilibrium structural properties across a large set of materials. Second, we introduce a workflow for the automatic optimization of local-orbital species files, significantly reducing the manual effort required to generate accurate basis sets for all-electron calculations. Finally, we highlight a high-throughput convergence workflow for Bethe–Salpeter equation (BSE) core-level spectroscopy, which automatically determines converged computational parameters for X-ray absorption spectra across a broad range of elemental solids. This workflow combines dynamic convergence strategies with automated recovery from failed calculations, enabling large-scale benchmark studies that would be impractical using conventional manual approaches.

To promote FAIR and reproducible computational research, `excitingworkflow` further enables the seamless publication of workflow results and complete provenance information directly to the NOMAD research data infrastructure, facilitating data sharing, reuse, and large-scale materials informatics.

Together, these examples demonstrate how workflow automation extends the applicability of all-electron methods to large materials datasets while preserving the high accuracy required for predictive electronic-structure and spectroscopy calculations. The presented framework establishes a foundation for future high-throughput studies and data-driven materials discovery using the `exciting` code.