# The FHI-aims Code and the GIMS Interface for Efficient, Precise All-Electron Simulations of Materials and Molecules

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This presentation and short tutorial introduces the FHI-aims code (https://fhi-aims.org/) [1] for all-electron electronic structure simulations of materials and molecules, as well as the browser-based Graphical Interface for Materials Simulations (GIMS, https://gims.ms1p.org) [2], which facilitates setup and analysis tasks of electronic structure based simulations in a simple, intuitive approach.

FHI-aims is the product of a very large, globally active community (over 150 contributing developers to date). The code builds on numeric atom-centered orbital basis sets, a prescription that enables all-electron simulations from fast qualitative to benchmark-quality numerical precision across the periodic table. Non-periodic and periodic simulation geometries are accessible on equal footing, with simulation sizes up to several thousand atoms based on semilocal and hybrid density functional theory (DFT), supported by computational scalability from laptops to supercomputers with ten thousands of CPU cores. Beyond ground-state DFT, many-body perturbation theory including *GW* and RPA (for non-periodic and periodic systems) as well as the Bethe-Salpeter Equation based on GW (for non-periodic systems) and real-time time-dependent DFT are supported by the code. Ongoing work includes GPU support (currently, for semilocal DFT), four-component relativistic methods, a frozen-core approach that accelerates large heavy-element containing simulations, and many other small and large additions from the broad community around FHI-aims. In the author's own environment, applications include hybrid DFT simulations of organic-inorganic hybrid perovskites with supercell sizes up to 1,500 atoms, of multinary chalcogenide semiconductors, molecular catalysts, surface science, and more. In short, FHI-aims enables a host of application areas throughout materials science, condensed-matter physics, chemistry, and related disciplines with precision, accuracy, and computational efficiency.

GIMS is an open-source, freely available, browser based graphical interface (no setup necessary) for molecular and materials simulations that currently supports two electronic structure codes (FHI-aims and exciting). Built upon widely used community software such as the Atomic Simulation Environment (ASE) and spglib, GIMS is designed to streamline essential setup and analysis tasks for electronic structure codes, deliberately designed to be extendable to further codes in the future.

A short introductory tutorial of how to handle molecular and periodic simulations, based on DFT and using FHI-aims and GIMS, completes this presentation.

## References

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