

**Title - Academic CASTEP in Practice: A Linux-Based Workshop on Installation, Computation, and Post-Processing**

**Short title - Academic CASTEP: A Practical Workshop**

**Abstract:**

Academic CASTEP - the Cambridge Serial Total Energy Package - is a plane-wave pseudopotential code for first-principles electronic structure calculations, distributed free of charge to academic institutions worldwide under the STFC licence. Although it is well established in the international research community, many students and researchers find that the practical side of the code presents a genuine obstacle: getting it compiled, configured, and running correctly on a Linux system is a non-trivial step that textbooks rarely address.

This one-day workshop is designed to close that gap. The goal is straightforward - participants leave with the ability to install, run, and post-process Academic CASTEP calculations on their own machines, independently and without relying on pre-configured environments.

The morning is devoted entirely to practice. Each participant boots a pre-configured Linux system from a live USB, compiles Academic CASTEP from source, and works through a complete calculation from scratch: writing input files, setting the essential parameters, submitting a job, and reading the output. The emphasis at this stage is on building confidence through direct experience rather than on formal theory.

The afternoon shifts toward productive and informed use of the code. Topics include convergence testing - energy cutoff and k-point sampling - pseudopotential selection and validation, and systematic post-processing using the CASTEP utilities suite to generate band structures, densities of states, and optical spectra. A focused section covers the practical implementation of DFT+U within CASTEP: specifying Hubbard projectors, assigning U values, and correctly interpreting the output, with particular attention to correlated systems such as transition metal compounds.

Participants who complete the workshop will be equipped to handle the full CASTEP workflow autonomously - from compilation through to publication-quality results - and will be ready to transfer that workflow to an HPC cluster running SLURM.

**Target audience:** PhD students and researchers with existing knowledge of DFT who wish to develop practical proficiency with Academic CASTEP. No prior experience with the code or with Linux is assumed.

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