

# CASTEP

A full-featured materials simulation package based on a quantum mechanical description of electrons and nuclei.

Technology No. 111

## Important notice

(Last update Monday 11th September 2023)

**It would be very helpful if licence applications provide complete information,** following our guidance alongside the licence questionnaire, and ensure that you follow your organisation's policy for legal acceptance of the licence terms when nominating your Authorised Representative.



[CASTEP](#) is a leading code for calculating the properties of materials from first principles. Using density functional theory, it can simulate a wide range of materials properties including energetics, structure at the atomic level, vibrational properties, electronic response properties etc. In particular it has a wide range of spectroscopic features that link directly to experiment, such as infra-red and Raman spectroscopies, NMR, and core level spectra.

Research groups can apply for a CASTEP academic source code licence, which is free-of-charge for non-commercial use. STFC ([CoSeC](#)) administers academic licences on behalf of [Cambridge Enterprise](#) and the [CASTEP Developers Group](#). Note that this academic licence only includes a command-line interface and does not include the [BIOVIA Materials Studio](#)-graphical interface.

Prospective commercial users can obtain CASTEP through the [BIOVIA Materials Studio](#)-product.

For further information, documentation, tutorials and community news, please visit <http://www.castep.org>.

Community support and archives can be found at the [CASTEP mailing list](#).

## Referencing CASTEP

In all papers using CASTEP please cite:

- [First principles methods using CASTEP](#), Zeitschrift für Kristallographie 220(5-6) pp. 567-570 (2005) S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson, M. C. Payne

Specific functionality may also require [additional citations](#).

Note that CASTEP will write a \*.bib file containing suitable references in a bibtex format at the end of a run.

## References

Clark, SJ; Segall, MD; Pickard, CJ; Hasnip, PJ; Probert, MJ; Refson, K; Payne, MC(2005), <https://doi.org/10.1524/zkri.220.5.567.65075>, <https://www.degruyter.com/view/journals/zkri/zkri-overview.xml>, 220; 5-6, 567-

570

<https://licences.stfc.ac.uk/product/castep>