

CASTEP

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

Important notice

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.

Category

Software/CASTEP

[View online](#)



[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 <https://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

1. 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