exciting News

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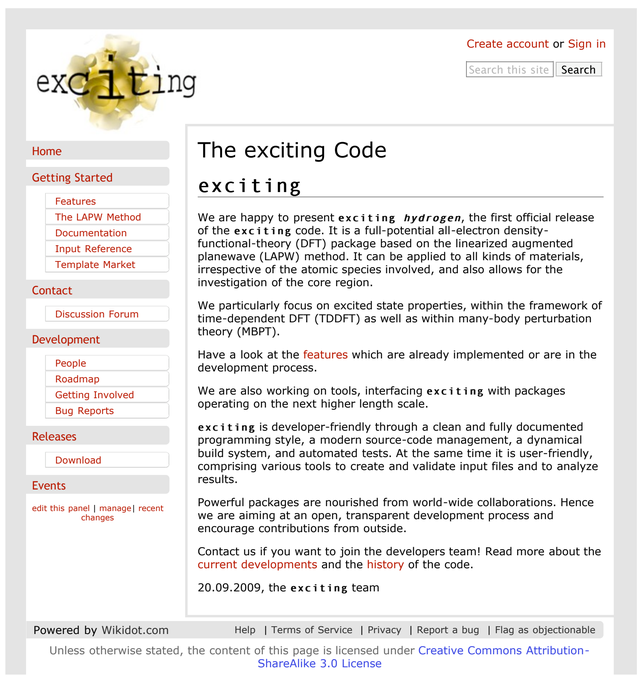
Abstract

The **exciting** code is a density-functional theory (DFT) and excited-states package based on the linearized augmented plane-wave (LAPW) method. It can be applied to all kinds of materials, irrespective of the atomic species involved, and also allows for the investigation of the core region. **exciting** is an open source code. The **exciting** *hydrogen* release can be obtained from `http://exciting-code.org`. The **exciting** project encourages contributions from the community. Automated tests, distributed version tracking, a flexible build system, online documentation, and the extensible XML input file format, form a solid basis for a distributed code development. Focusing on the latter, XML provides two basic advantages: One comes with the schema language, XML Schema, which allows for a formal description of the input file format. This schema can be used to validate the input file with standard validation tools. In addition, one can generate documentation, parsing code, and an user interface from one source. Being machine and human readable, XML is the optimal file format for data output as well. Application specific file formats are then generated in a separate step through templates. All these ideas are exploited in the **exciting**@web database, a newly developed software suited to publish DFT data on the internet and also providing an interactive interface to the **exciting** code.

Website

http://exciting-code.org

- Tutorials
- Input reference
- Example code
- Templates
- Developer resources
- Forum
- Mailing list
- Downloads



Features

General

- High precision all-electron DFT code based on the FP-LAPW method including local-orbitals
- Various XC functionals available
- Calculation of forces and structural optimization
- Treatment of magnetism in the most general way, including spin-orbit coupling and non-collinear magnetism
- Plotting of band structure, Fermi surface, charge density, potential etc. (1D, 2D and 3D)
- Visualization with xmgrace and XCrySDen supported
- MPI parallelization, as well as optimization for multithreaded numeric libraries (BLAS LAPACK)
- Simple to use: just one input file required
- XML inputs / outputs

Excited states

- Macroscopic dielectric function within time-dependent DFT and the Bethe-Salpeter equation
- Available exchange-correlation kernels: RPA, ALDA, long-range contribution model-kernels, BSE-derived kernel
- RPA and ALDA loss function for finite momentum transfer q-vectors

Programming

- Clean and simple code structure – ideal for development
- Git repository
- Full LaTeX documentation included with every subroutine

LAPW

In the linearized augmented plane-wave (LAPW) method the unit cell of the crystal is divided into two different types of regions. The first one, called the muffin-tin region, consists of spheres centered around the atoms, while the second one, called the interstitial region, consists of the remaining part of the unit cell. In the muffin-tin spheres the basis consists of atomic like functions to account for the rapid changes of the wave function in this area, whereas in the interstitial region the basis functions are plane waves, since the wave function changes only slowly at some distance from the atomic sites.

$$\phi_{\mathbf{p}}(\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} e^{i\mathbf{p}\mathbf{r}}, & \mathbf{r} \in \mathrm{I} \\ \sum_{lm}^{\mathrm{lmax}} f_{lm}^{\alpha}(|\mathbf{r}-\mathbf{R}_\alpha|;\mathbf{p}) Y_{lm}(\widehat{\mathbf{r}-\mathbf{R}}_\alpha), & \mathbf{r} \in \mathrm{MT}_\alpha \end{cases}$$

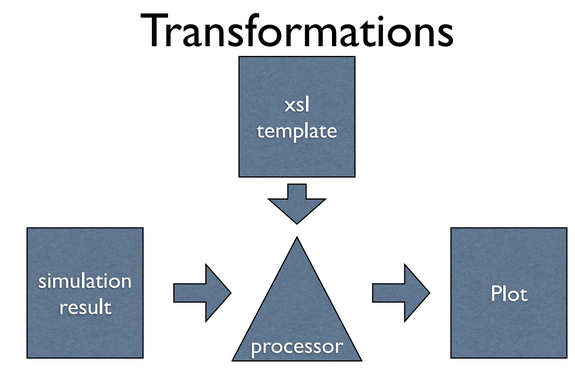
The LAPW basis set is specially designed to describe the wave function of all electrons in the full potential of a periodic solid, which makes it a highly accurate method and also allows for the investigation of the core region.

Current Developments

- Stress tensor (Pasquale Pavone)
- Elastic properties (Pasquale Pavone)
- Phonon dispersion (Stephan Sagmeister)
- Van der Waals density functional (Dmitrii Nabok)
- k.p@LAPW (Jürgen Spitaler in collaboration with, KTH Stockholm)
- ATAT@exciting (Jürgen Spitaler)
- GW (collaboration with FHI Berlin)
- Graphical user interface (Christian Meisenbichler)

XML Output

exciting writes data in XML format. These XML files may be transformed to many target formats using XSLT. **exciting** comes with a selection of XSLT templates e.g. for inputs to visualization tools. XSLT is a language specifically designed for that purpose. Therefore templates can be developed very efficiently.



Definitions

XSLT, the XML Stylesheet Language Transformations [1], is a language designed to transform XML into other formats with so called templates. It is in itself expressed in XML and is a functional, declarative language.

XForms is a W3C recommendation for creating forms on XML data [2]. It is an embedded language with XML syntax. The rendering of the forms in a web page may be done with a browser plugin or by translating it into HTML and javascript by an application on the server. XSLTForms is one way to do this.

XSLTForms is a template and a javascript library that allows for rendering XForms in HTML and javascript [3].

XML Schema is a schema language for XML. It allows to define the grammar and datatypes of an XML file format.

XML Databases such as exist-db [4] are applications designed to efficiently store and query XML data. The standard query language is XQuery.

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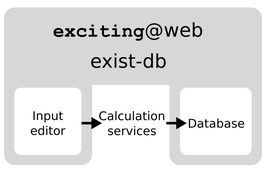
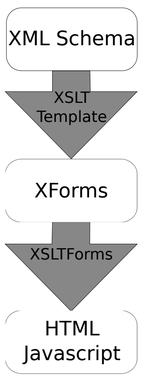
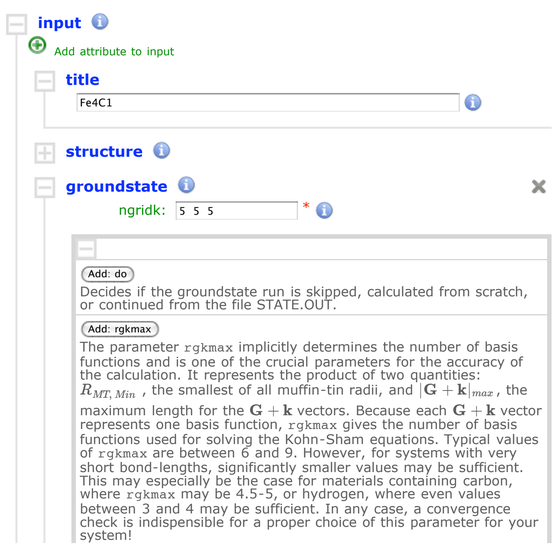
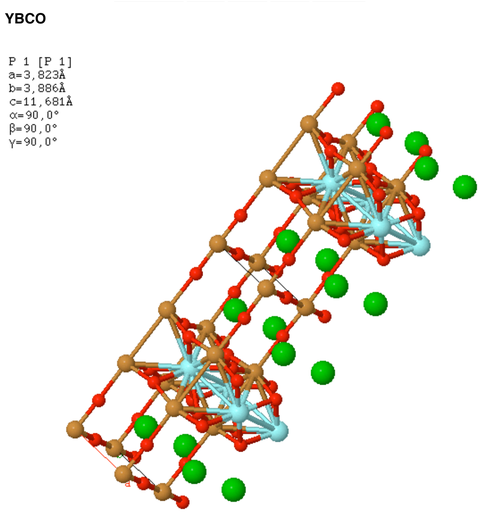


The **exciting**@web application consists of a GUI to edit and create **exciting** input files, an interface to submit and monitor **exciting** calculations, as well as a database to store, query, and visualize data.
The graphical user interface (GUI) is generated from the XML Schema of the **exciting** input file. The Schema is used to generate XForms code with a custom XSLT style sheet. This XForms code is transformed to HTML by the XSLTForms XSLT style sheet. The generation of the GUI from the schema has the advantage that it keeps the GUI up to date with the development of the **exciting** code automatically.

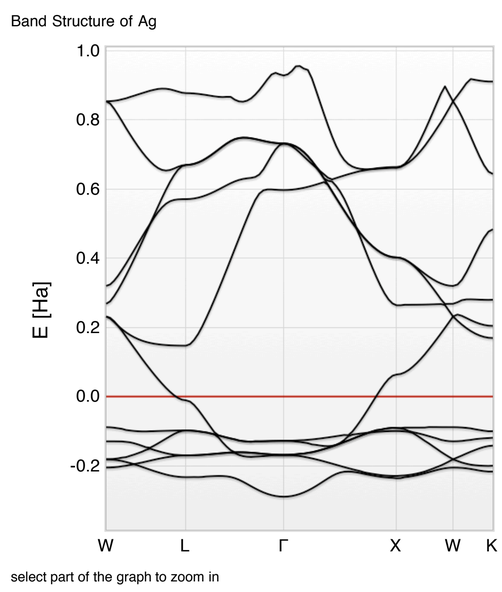




exciting@web provides an interactive input file editor (GUI). It can add elements and attributes without reloading the page. The elements and attributes are selected from collapsible panels which show the possible choices along with the documentation. The result is an interactive application that guides the user through setting up the input.
The input editor can load any valid input file. It covers all the functionality of the code, because it is automatically generated from the schema.



The **exciting**@web database provides a special view on the **exciting** input file. This view includes visualization of 3D structures using `Jmol`. The used input parameters are listed and linked to their description in the documentation.



Important graphs such as bandstructure and density of states are directly rendered in the browser. In addition, one can download the picture in other file formats. New file formats can be added by associating the XML data file with an XSLT template that performs the format conversion.

Acknowledgements

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References

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