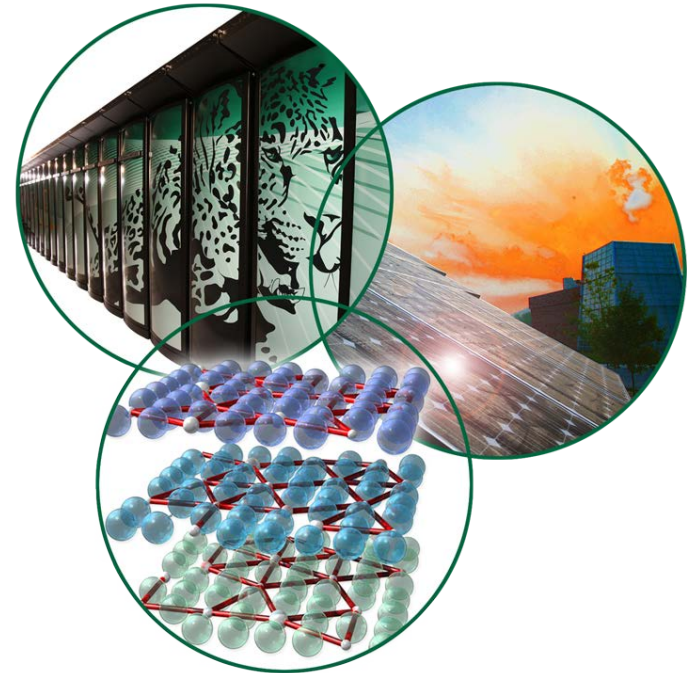


Important software tools for magnetic structure determination

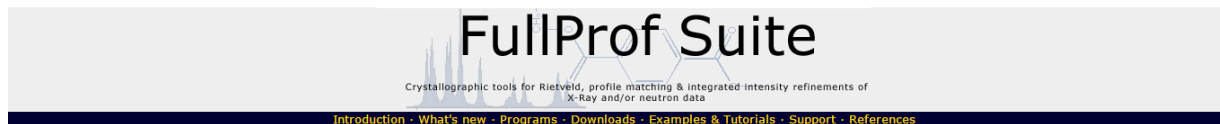
*Ovidiu Garlea
Quantum Condensed Matter Division
Oak Ridge National Laboratory*

- Rietveld packages
- Creating magnetic models:
 - Symmetry analysis tools
- Visualization tools



□ Rietveld packages that can refine magnetic structures

FullProf_Suite: <https://www.ill.eu/sites/fullprof/>



The FullProf Suite (for Windows and Linux) is formed by a set of crystallographic programs (FullProf, WinPLOTR, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2θ .

The different programs can be run either in stand alone form (from a console window or clicking directly in a shortcut) or from the interfaces WinPLOTR and/or EdPCR.

The programs within the FullProf Suite are distributed in the hope that they will be useful, but WITHOUT ANY WARRANTY of being free of internal errors. In no event will the authors (or their institutions) be liable to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the programs (including but not limited to loss of data or data being rendered inaccurate or losses sustained by you or third parties or a failure of the program to operate with any other programs). The authors are not responsible for erroneous results obtained with the programs.

JANA: <http://jana.fzu.cz/>

A screenshot of the JANA website homepage. The browser address bar shows "jana.fzu.cz". The main content area features a large, stylized logo of the word "JANA" inside a circular, textured frame. To the right of the logo is contact information for the Institute of Physics, Department of Structure Analysis, located at Cukrovarnicka 10, 16253 Praha 6, Czech Republic. Below this is a section titled "CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES" by Vaclav Petricek, Michal Dusek & Lukas Palatinus. A "News" section lists several updates, including a deadline for abstract submission to ECM30 in Basel, Switzerland, and a maintenance release of Jana2006 for Windows.

GSAS/ EXPGUI: <https://subversion.xray.aps.anl.gov/trac/EXPGUI>

https://subversion.xray.aps.anl.gov/trac/EXPGUI

Welcome to the EXPGUI Trac site

This is a web system for access to the EXPGUI package, to log problems with the package, and to see what has been changed. GSAS & EXPGUI should be downloaded with links here. Downloads from non-Argonne servers may be long out of date. Note there are several distribution mechanisms available for installation.

Installation notes:

See [Windows](#), [Mac OS X](#), or [Linux](#) for details on how to install.

EXPGUI links:

- documentation: <https://subversion.xray.aps.anl.gov/EXPGUI/trunk/doc/expgui.html>
- mailing list: <http://www.aps.anl.gov/mailman/listinfo/expgui>
- subversion server address: <https://subversion.xray.aps.anl.gov/EXPGUI/>
- EXPGUI project tracking: <https://subversion.xray.aps.anl.gov/trac/EXPGUI/> (here)

GSAS & EXPGUI links:

- Introductory information about GSAS
- distributions: <http://t3lib.xray.aps.anl.gov/download/gsas>
- new installation instructions: [Windows](#), [Mac OS X](#), or [Linux](#)
- GSAS Manual: <https://subversion.xray.aps.anl.gov/EXPGUI/gsas/all/GSAS%20Manual.pdf>
- APS training lectures: http://www.aps.anl.gov/Xray_Science_Division/Powder_Diffraction_Crystallography/
- GSAS/EXPGUI Tips

GSAS-2 : <https://subversion.xray.aps.anl.gov/trac/pyGSAS>

https://subversion.xray.aps.anl.gov/trac/pyGSAS

GSAS-2

GSAS-II Home

GSAS-II is an open source Python project that addresses all types of crystallographic studies, from simple materials through macromolecules, using both powder and single-crystal diffraction and with both x-ray and neutron probes. Measurements can be constant wavelength or TOF (thanks to support from Oak Ridge National Lab.) GSAS-II supports everything that GSAS/EXPGUI does, except for magnetic scattering, but GSAS-II also handles all the steps in diffraction analysis, such as data reduction, peak analysis, indexing, Pawley fits, small-angle scattering fits, structure solution in addition to structure refinement. It can be used with large collections of related datasets for repeated (sequential) refinements and for parametric fitting to these results. The source code can be found at <https://subversion.xray.aps.anl.gov/pyGSAS/trunk/>

The code is changing on a regular basis, so expect things to break from time to time (see bug reporting, [below](#)). Be sure to 'update' frequently to stay abreast of new features as they are added.

If you use GSAS-II, please sign up for the GSAS-II mailing list, see web page <http://www.aps.anl.gov/mailman/listinfo/GSAS-II> and **please cite it**.

Installation instructions

- [Windows](#)
- [Mac OS X](#)
- [Linux](#)

RIETAN : http://fujiioizumi.verse.jp/download/download_Eng.html

fujiioizumi.verse.jp/download/download_Eng.html

Distribution Files for the RIETAN-FP-VENUS Package

We have been developing programs to analyze crystal structures from X-ray and neutron powder diffraction data and visualize results of the analyses as well as electronic-state calculations in three dimensions. Through distribution of these programs free of charge, we wish to promote quantum-beam technology and work on a social action program of [NIMS](#).

This Web page allows you to download two archive files for Windows 7/8 and OS X 10.6 (Snow Leopard) or later. Each of them contains Fortran programs listed below, examples of their execution, an integrated assistance environment for RIETAN-VENUS, PDF manuals, etc.

1. A multi-purpose pattern-fitting system RIETAN-FP v2.81 (the successor to RIETAN-2000)
2. ORFFE to calculate geometrical parameters from lattice and structure parameters resulting from Rietveld analysis with RIETAN-FP
3. `IntCrd` to convert *.`int` (standard output of RIETAN-FP) plus `dir` (standard output of ORFFE) into *.`cif`
4. An acrobatic bash script, `MPF_multi` command, for automatic MPF analyses
5. `ALBA` to analyze diffraction data by the maximum-entropy Patterson method
6. MADEL to calculate site potentials and Madelung energies from lattice and structure parameters

In MEM-based pattern fitting (MPF), RIETAN-FP and `Dynosmia` are alternately executed while examining distribution of electron or nuclear densities resulting from MEM analysis. With `MPF_multi` command, two or more MPF analyses, where standard uncertainties of F_o are adjusted as specified by the user, can be executed automatically.

[VESTA](#) (the successor to VICES and VENDOR) and `Dynosmia` (the successor to PRDIMA) in the `VENUS` system are distributed in [JP-Minerals](#).

The assistance environments for Windows and OS X, respectively, function on two major text editors, `Hedemans Editor` and `JeditX`, popular in Japan.

□ Symmetry analysis tools for creating magnetic models:

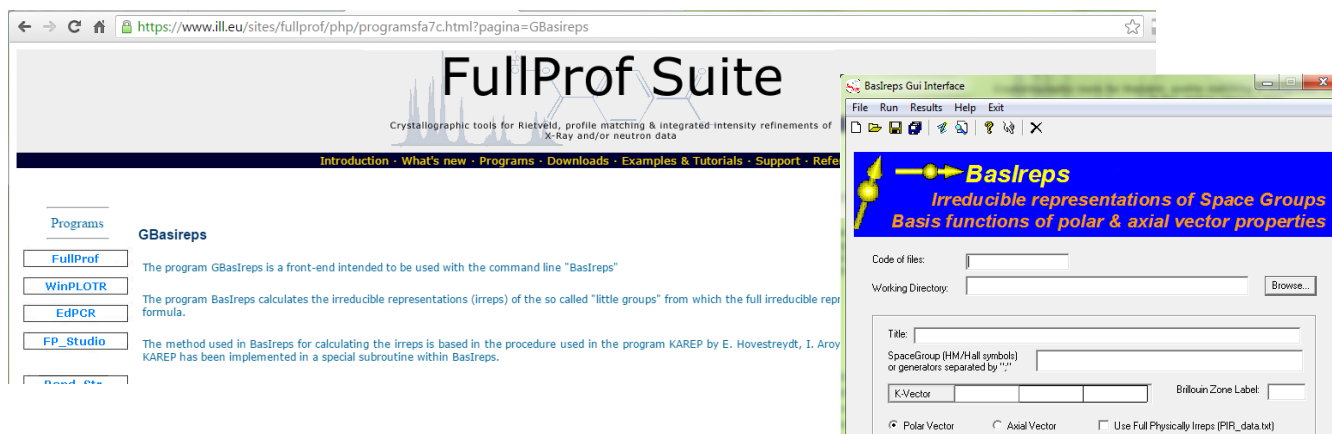
SARAh Representational Analysis:

<https://dl.dropboxusercontent.com/u/8933134/Website/Site/Software/Software.html>

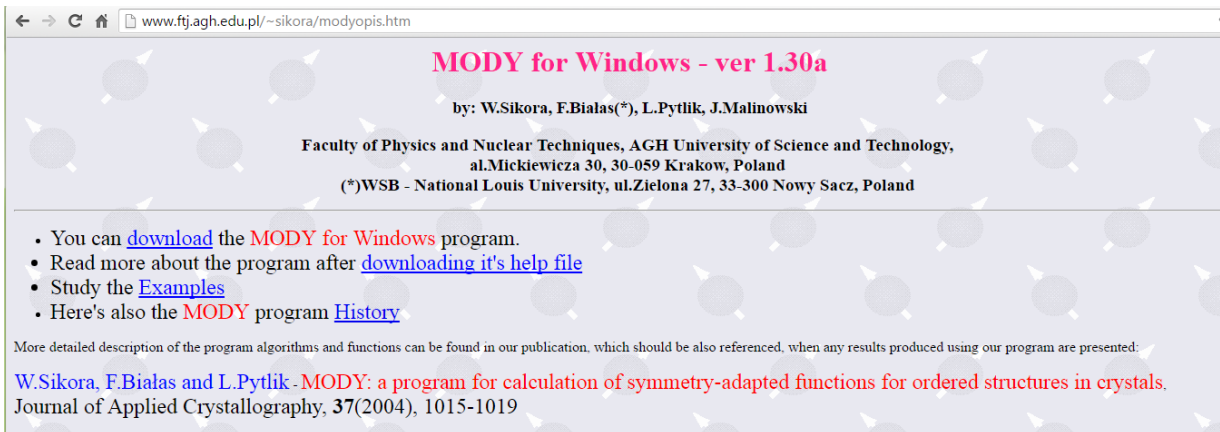


Basireps (FullProf_Suite)

<https://www.ill.eu/sites/fullprof>



MODY: <http://www.ftj.agh.edu.pl/~sikora/modyopis.htm>



A screenshot of a web browser showing the MODY program page. The browser address bar displays "www.ftj.agh.edu.pl/~sikora/modyopis.htm". The page title is "MODY for Windows - ver 1.30a". Below the title, it lists the authors: "by: W.Sikora, F.Bialas(*), L.Pytlík, J.Malinowski". The affiliation is "Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, al.Mickiewicza 30, 30-059 Krakow, Poland" and "(*)WSB - National Louis University, ul.Zielona 27, 33-300 Nowy Sacz, Poland". A list of links includes "download", "downloading it's help file", "Examples", and "History". A paragraph of text mentions a publication: "W.Sikora, F.Bialas and L.Pytlík - MODY: a program for calculation of symmetry-adapted functions for ordered structures in crystals, Journal of Applied Crystallography, 37(2004), 1015-1019".

MAGMAX: [Bilbao Crystallographic Server](http://www.cryst.ehu.es/cgi-bin/cryst/programs/msglist2.pl)

<http://www.cryst.ehu.es/cgi-bin/cryst/programs/msglist2.pl>



A screenshot of the Bilbao Crystallographic Server interface for the MAXMAGN program. The browser address bar shows "www.cryst.ehu.es/cgi-bin/cryst/programs/msglist2.pl". The page title is "MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models". A blue box contains the program description: "MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models". Below this, a paragraph explains: "MAXMAGN provides the possible magnetic space groups that can be assigned to a 1-k commensurate magnetic phase assuming that the magnetic symmetry is a maximal one. The space group of the paramagnetic phase (parent group) and the observed propagation vector are required as input. Optionally, the parent paramagnetic structure can be". To the right, there are two checkboxes: "Structure data of the paramagnetic phase will be included" and "Non-conventional setting". Below these are two input fields: "Please, enter the label of the space group of the paramagnetic phase (parent group)" with a "choose it" button, and "Please, enter the propagation vector k:" with input boxes for k_x , k_y , and k_z .

ISOTROPY Software Suite: <http://stokes.byu.edu/iso/isotropy.php>

← → ↻ 🏠 stokes.byu.edu/iso/isotropy.php

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- **ISODISTORT:** Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- **New! ISOSUBGROUP:** Interactive program using user-friendly interface to list isotropy subgroups.
- **ISOTROPY:** Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- **SMODES:** Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- **FROZSL:** Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations

- **ISOCIF:** Create or modify CIF files.
- **FINDSYM:** Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **ISO-IR:** Tables of Irreducible Representations. The 2011 version of IR matrices.
- **ISO-MAG:** Tables of magnetic space groups, both in human-readable and computer-readable forms.

Neutron Sciences



Mag. Str. Workshop – 2016, Tallahassee, FL



Visualization tools:

FPStudio:

https://www.ill.eu/sites/fullprof/php/programs71b4.html?pagina=FP_Studio

The image shows two side-by-side screenshots. On the left is the website for FullProf Suite, which includes a navigation menu with buttons for 'FullProf', 'WinPLOTR', 'EdPCR', 'FP_Studio', and 'Bond_Str'. The main content area features the title 'FullProf Suite' and a description of the software as 'Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data'. On the right is a screenshot of the FPStudio software interface, displaying a 3D visualization of a crystal structure with atoms represented by spheres and bonds shown as lines.

MVISUALIZE: [Bilbao Crystallographic Server](http://webbdcrista1.ehu.es/magndata/mvisualize.php)

<http://webbdcrista1.ehu.es/magndata/mvisualize.php>

http://webbdcrista1.ehu.es/magndata/mvisualize.htm?newcif=CuMnO2_45644.png&produced=tmp/mvisualize_45644.mcif&mcif=1j8DcmVhdGVkIGV5HRozS8CawWYw8qQ

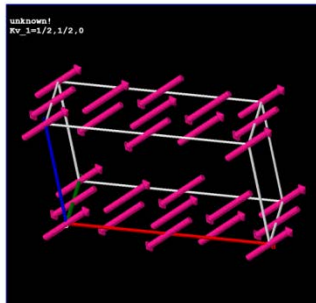
MVISUALIZE: 3D Visualization of magnetic structures with Jmol

MVISUALIZE Main Page

Download complete mcif file (including all tags needed for submission to MAGNDATA)

Show File

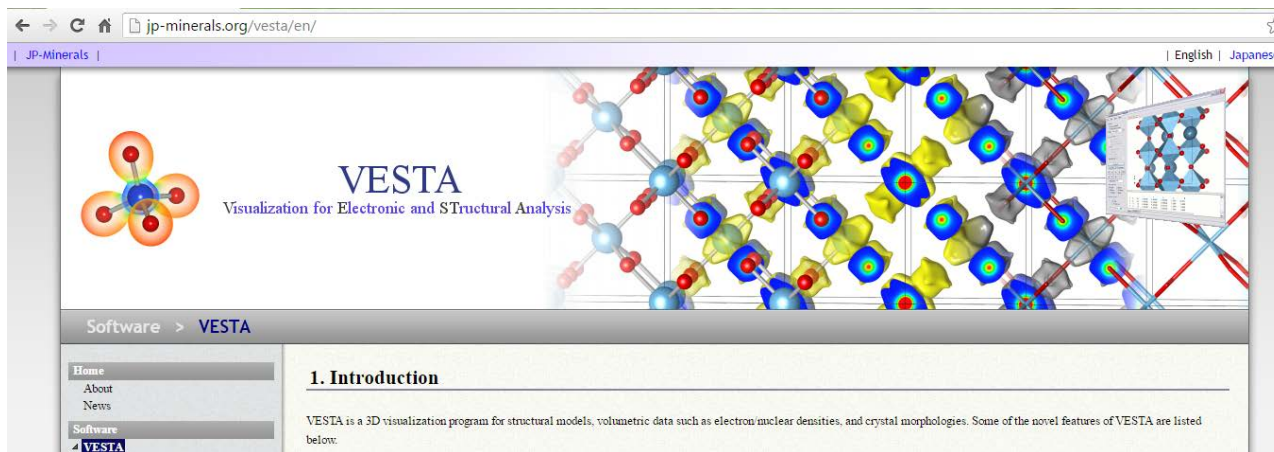
Change setting



A control panel for the 3D visualization of magnetic structures. It includes various options and settings:

- Working Cell: Toggle Panel Cell, Toggle Standard Cell
- View Along Axis: Unit Cell Info
- All / Magnetic Atoms: Show/Hide Labels
- Larger / Smaller: Vectors, Larger / Smaller: Atoms
- Window Size: Bigger, Smaller
- Background Color: Center
- Export PNG Image: Save PNG-3D, Save ZIP file
- Show unit cell a,b,c: Add 1 cell along x, Remove 1 cell along x, Add 1 cell along y, Remove 1 cell along y, Add 1 cell along z, Remove 1 cell along z
- Draw bonds & polyhedra: Join, with, from 0.75 to 2.75, A
- Draw: Bonds, Polyhedra, Delete: Bonds, Polyhedra, Clear all drawings

VESTA: <http://jp-minerals.org/vesta/en/>



VESTA
Visualization for Electronic and Structural Analysis

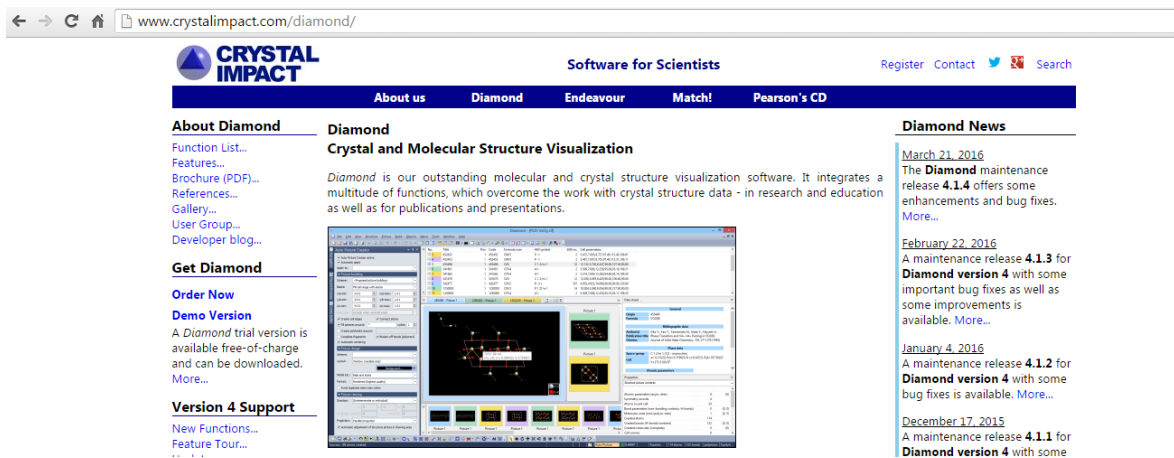
Software > VESTA

Home
About
News
Software
VESTA

1. Introduction

VESTA is a 3D visualization program for structural models, volumetric data such as electron nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below:

Diamond: <http://www.crystalimpact.com/diamond/>



CRYSTAL IMPACT
Software for Scientists
Register Contact Search

About us Diamond Endeavour Match! Pearson's CD

About Diamond

Function List...
Features...
Brochure (PDF)...
References...
Gallery...
User Group...
Developer blog...

Get Diamond

Order Now
Demo Version
A Diamond trial version is available free-of-charge and can be downloaded. More...


Version 4 Support

New Functions...
Feature Tour...

Diamond

Crystal and Molecular Structure Visualization

Diamond is our outstanding molecular and crystal structure visualization software. It integrates a multitude of functions, which overcome the work with crystal structure data - in research and education as well as for publications and presentations.



Diamond News

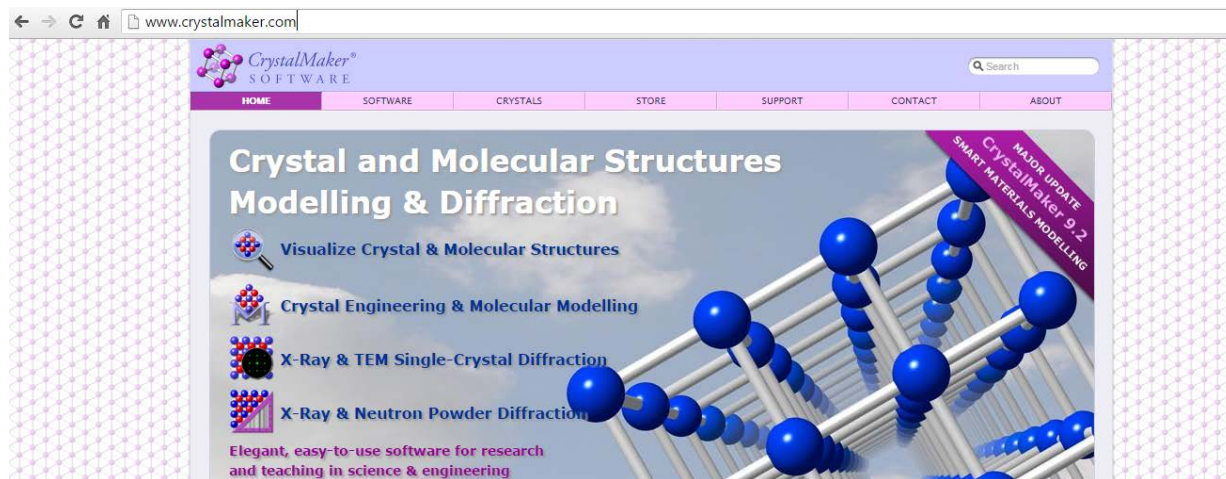
March 21, 2016
The **Diamond** maintenance release **4.1.4** offers some enhancements and bug fixes. More...

February 22, 2016
A maintenance release **4.1.3** for **Diamond version 4** with some important bug fixes as well as some improvements is available. More...

January 4, 2016
A maintenance release **4.1.2** for **Diamond version 4** with some bug fixes is available. More...

December 17, 2015
A maintenance release **4.1.1** for **Diamond version 4** with some

CrystalMaker: <http://www.crystallmaker.com/>



SpinW: <https://www.psi.ch/spinw/>

