

Installation notes

For the workshop, following programs are necessary:

PETS2 for data processing of electron diffraction patterns

Vesta for visualization of structure and 3D density of electrostatic potential

Jana2020 for most tasks

Superflip (part of Jana2020 distribution) for solution of phase problem

MCE (part of Jana2020 distribution) for visualization of 3D electrostatic potential.

Installation of PETS2

Download the latest version of PETS2 from <http://pets.fzu.cz>.

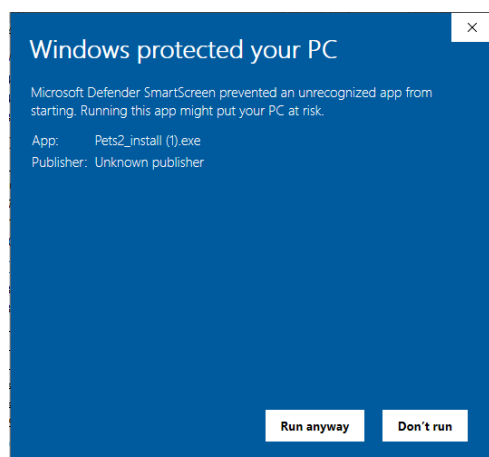
PETS2 Downloads	
link to the page with the installer (free registration required)	go to login page
manual	download

It is necessary to register with your email.

Download the latest version.

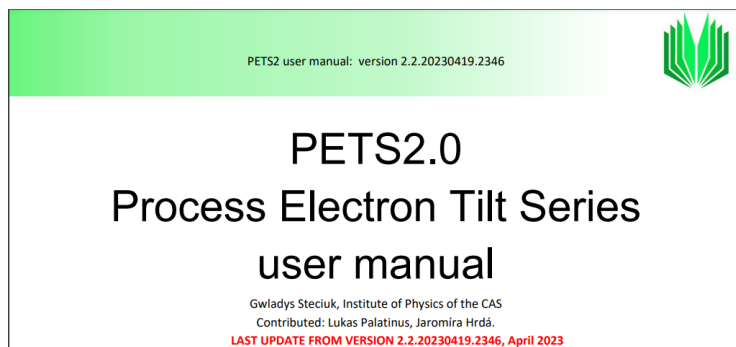
Versions
The latest version of PETS2: 27/05/2023 build 2.2.20230527.0801
Download Latest version

Execute the exe file to install PETS2. In case you run the exe file from a browser, you may be asked if the installed software is safe. Press „more details“ and „run anyway“.



Keep the default settings.

Download also the manual.

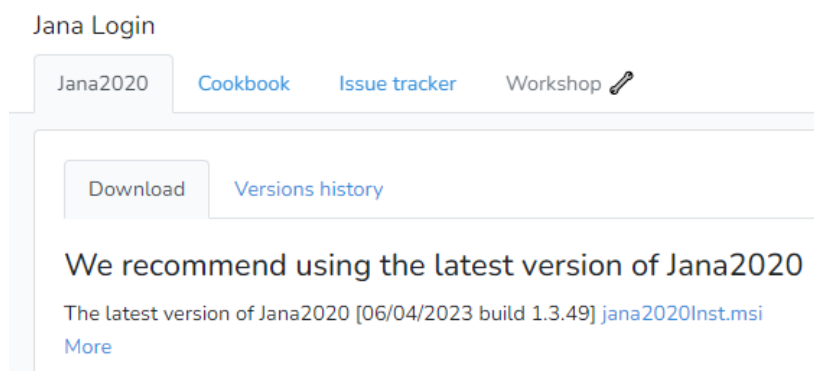


Installation of Vesta

Download the latest version from <https://jp-minerals.org/vesta/en/download.html>. Extract the zip file to a directory of your choice.

Installation of Jana2020

Download the latest version from <https://jana-login.fzu.cz/login>. You have to register with your email.



Execute janainst.msi and follow instructions. Don't use your "old" preinstalled versions of Jana2006/2020. Don't use flash disk for calculation. Go to "Help → About Jana2020" and verify the version string. The version date should be close to the workshop date.

Configuration of Jana2020

Start Jana2020 Go to "Settings → Programs"; leftclick with mouse the textbox "Graphic viewer"; press "Browse" and localize VESTA.exe. Leftclick in "3d visualization of maps"; press "Browse" and localize VESTA.exe. For using a different text editor than Notepad define its pathname in the textbox "Editor name".

Examples PETS2 for accurate lattice parameters download

Raw data and PETS2 input files for examples 1 and 2.

Link <https://doi.org/10.5281/zenodo.6424241>

Manuals for Examples 1 and 2: Part S4 in

DOI: <https://doi.org/10.1107/S2052252522007904/zu5001sup1.pdf>

Examples PETS2 + Jana2020 data reduction, structure solution and refinement download

Tutorials PETS2 + Jana2020

quartz	tutorial text	data
glycine	tutorial text	data
borane B18H22	tutorial text	data
abiraterone acetate	tutorial text	data
Ni ₂ Si	tutorial text	data
orthopyroxene	tutorial text	data
paracetamol	tutorial text	data
pyrite	tutorial text	data

Easy/beginner examples: quartz, glycine, abiraterone acetate, Ni₂Si.

Intermediate examples: borane, orthopyroxene, paracetamol, pyrite.