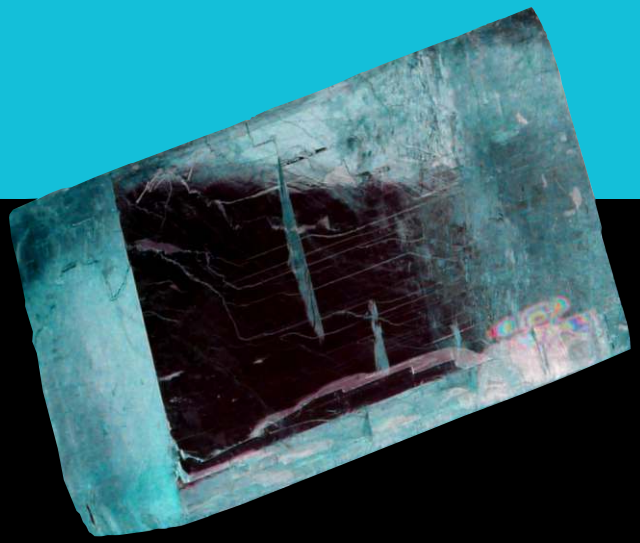
atomic matters

atomic properties and magnetism of solids

atomic matters MFA

Mean Field Approximation atomic computation system



Explore the features and functionality of ATOMIC MATTERS & ATOMIC MATTERS MFA computation systems. The following screenshots present relevant examples of the functional algorithm which should help you comprehend the software interface and principles.

ATOMIC MATTERS is designed to calculate, simulate and visualize the most relevant properties of materials which are determined by the fine electronic structure of contained ions or atoms in defined conditions.

ATOMIC MATTERS MFA is software for magnetic phase transition simulation according to Mean Field Approximation methodology.

The synergy of both applications makes it possible to predict the macroscopic properties of materials in user-defined temperature regions by using the physical properties of atomic electron systems under the influence of an external magnetic field. The software systems are intuitive and productive due to their graphical user interface, the wealth of interactive tools including 3D interactive visualizations, and the easy portability of data.

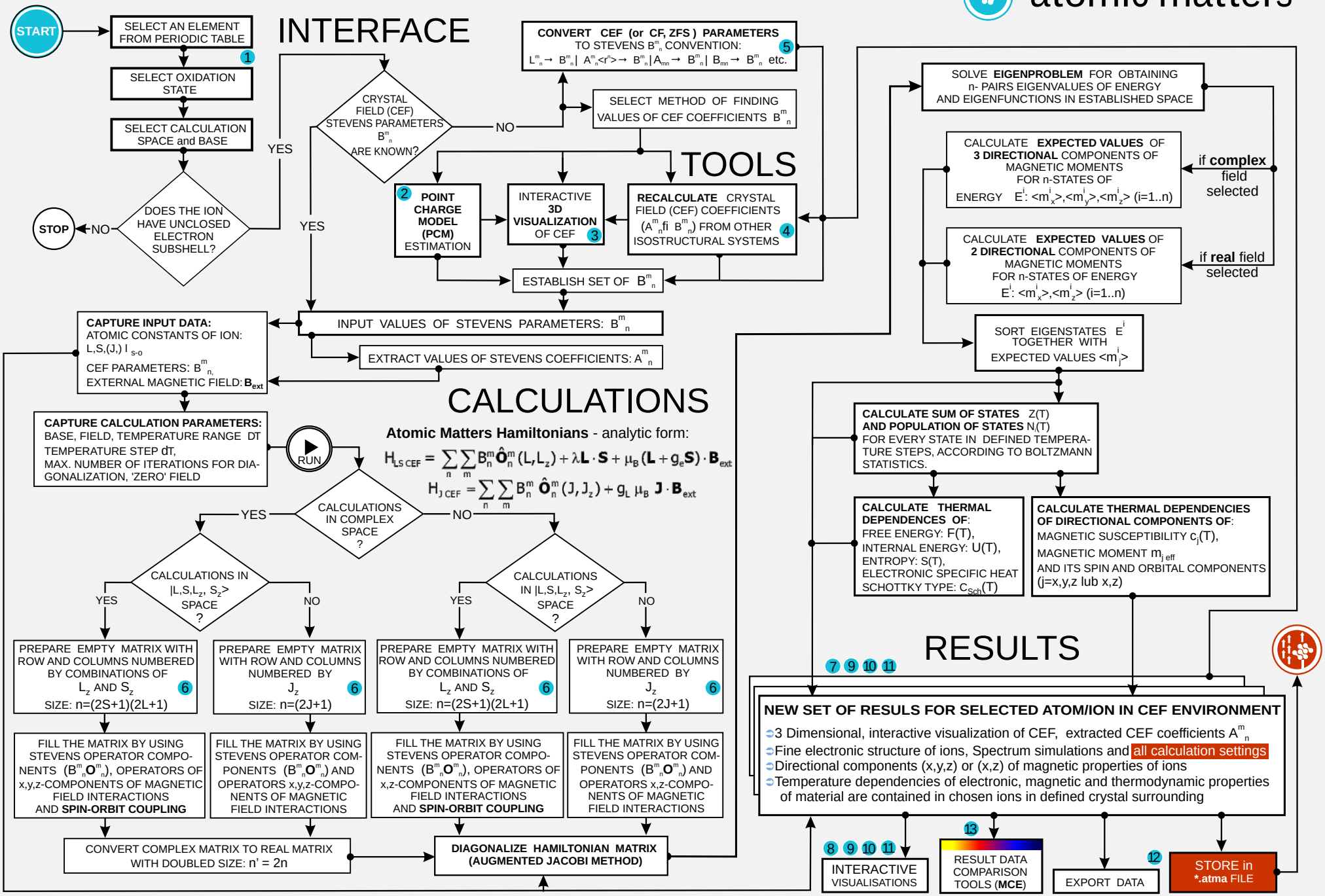
JOIN US TO TEST AND DEVELOP
ATOMIC MATTERS SOFTWARE

Rafał Michalski

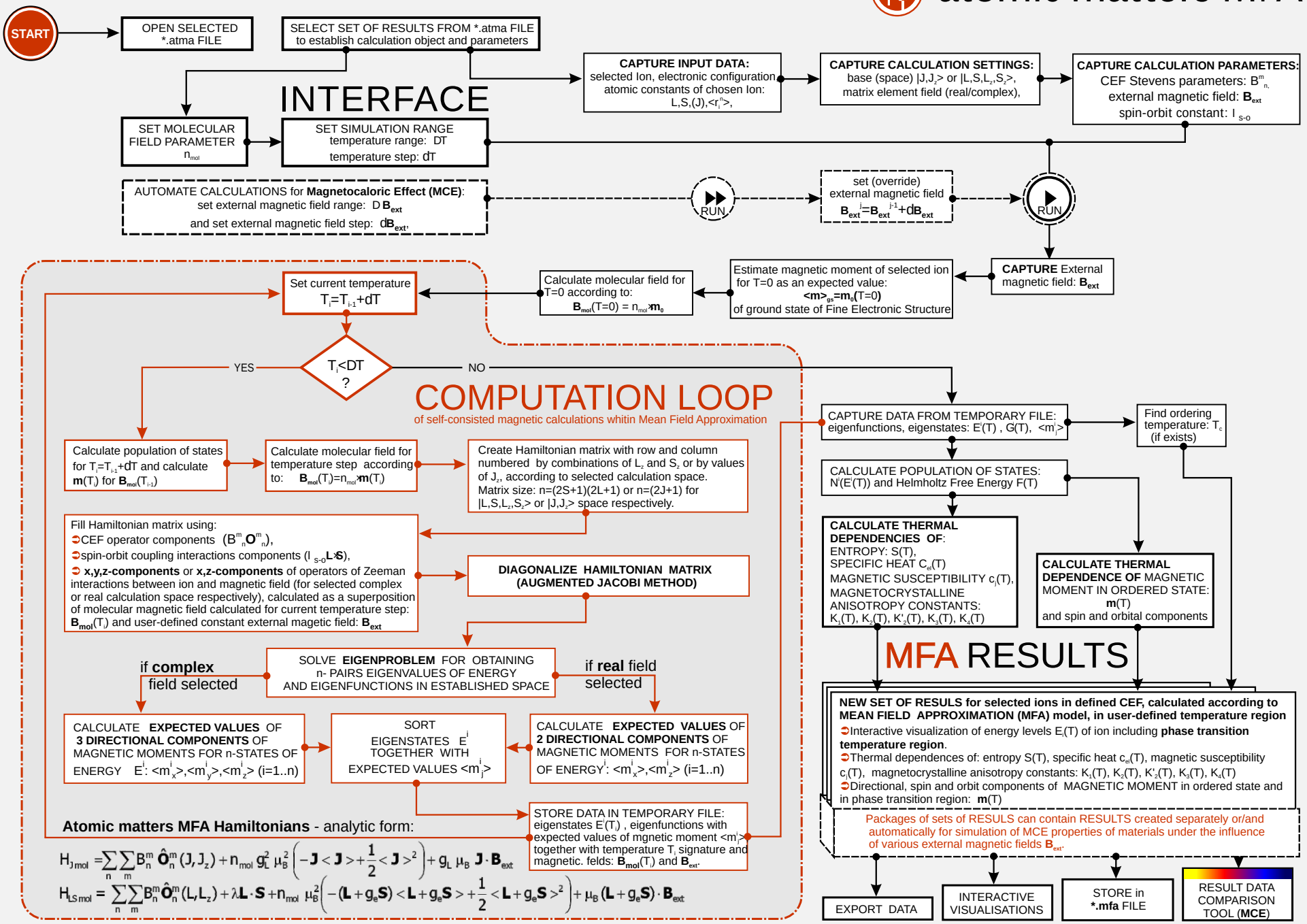
Atomic Matters project Leader

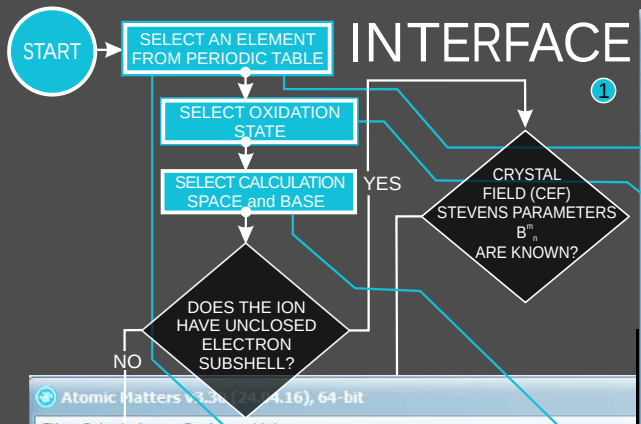
atomic matters BLOCK DIAGRAM of aplication

atomic matters



atomic matters MFA





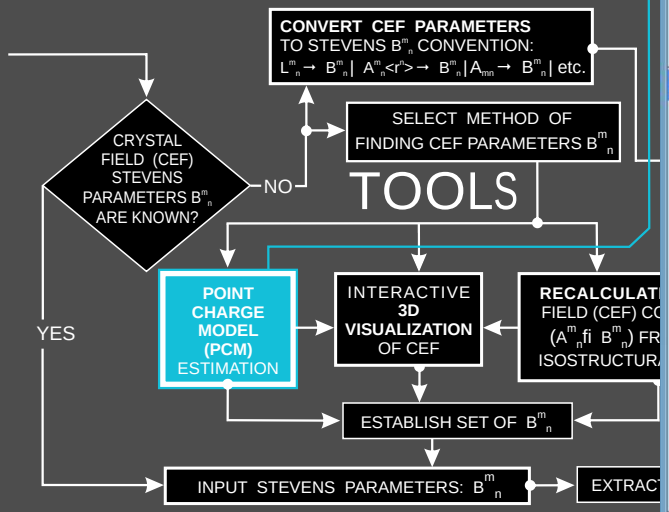
ESTABLISHING
OBJECT OF CALCULATIONS

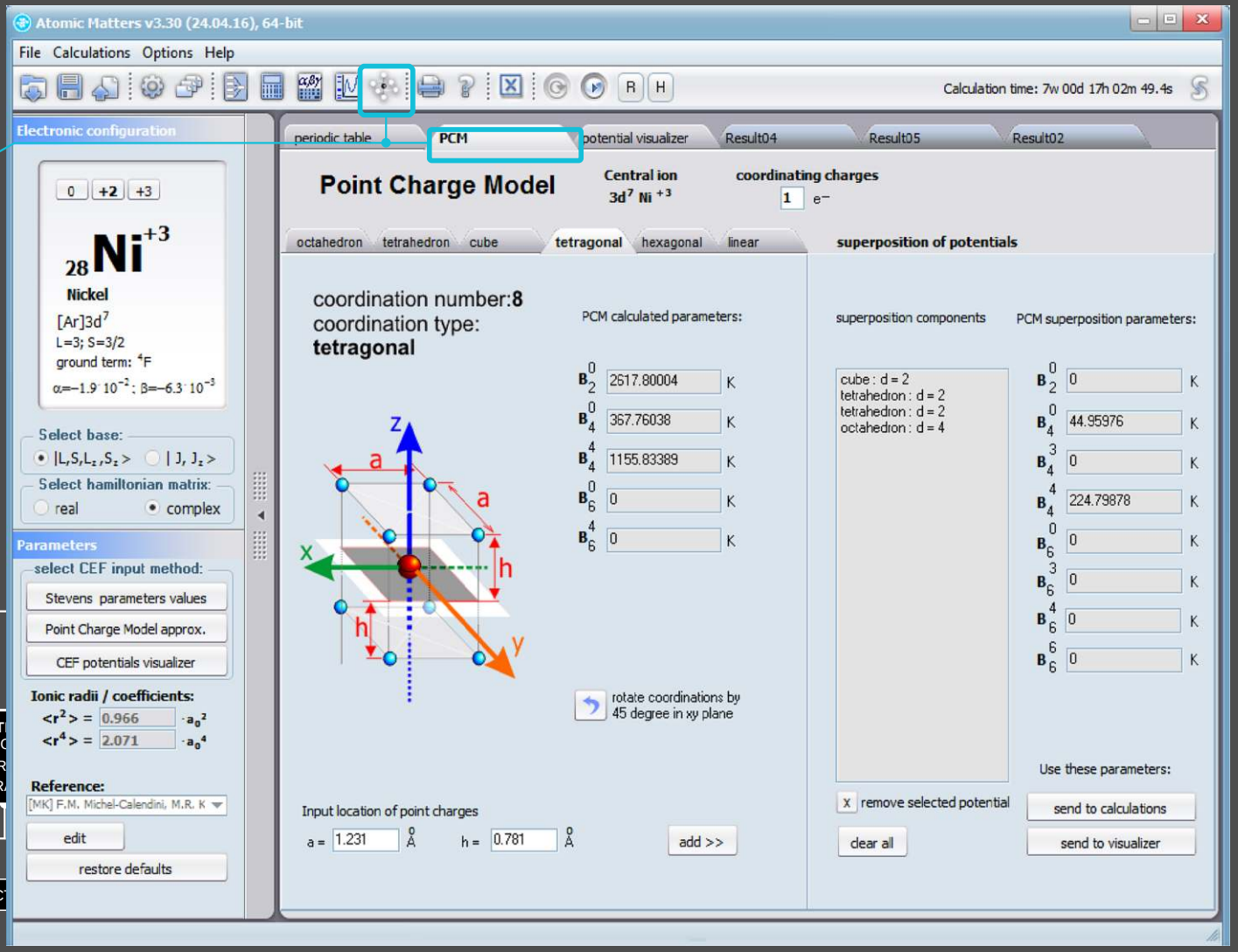
Select an Element from Periodic Table. Set oxidation state of chosen ion. Select calculation base and field for Hamiltonian matrix elements. Decide how to estimate Crystal Electric Field (CEF) parameters. *.atma files can be loaded to set desired ion and CEF configuration.

② PCM CALCULATOR
POINT CHARGE MODEL APPROXIMATION

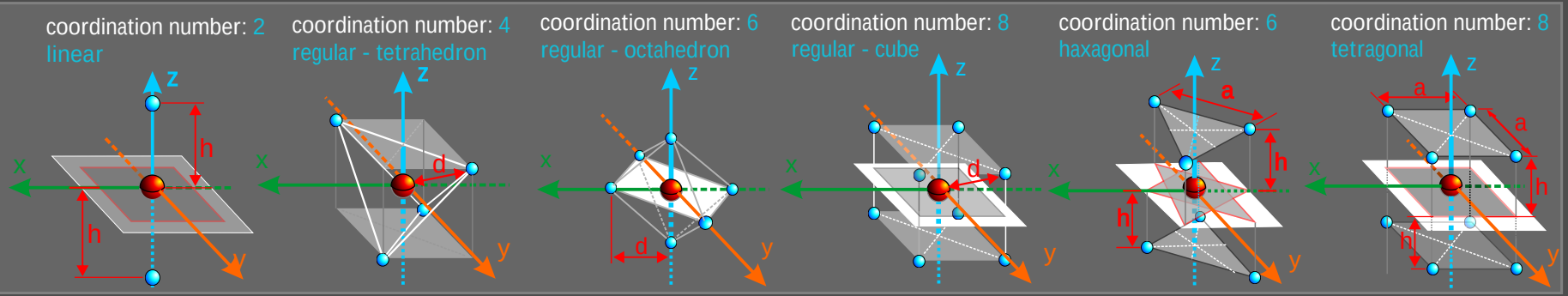
TOOLS

Point Charge Model approximation is a useful calculation technique for finding Crystal Field (CEF) parameters.
PCM calculations have never been so easy!
Choose spatial distribution of point charges by adding highly-symmetrical structures with charges a defined distance from the central ion.
CEF parameters obtained this way can be sent directly to the Input Parameter tab or visualized in the Potential Visualizer.



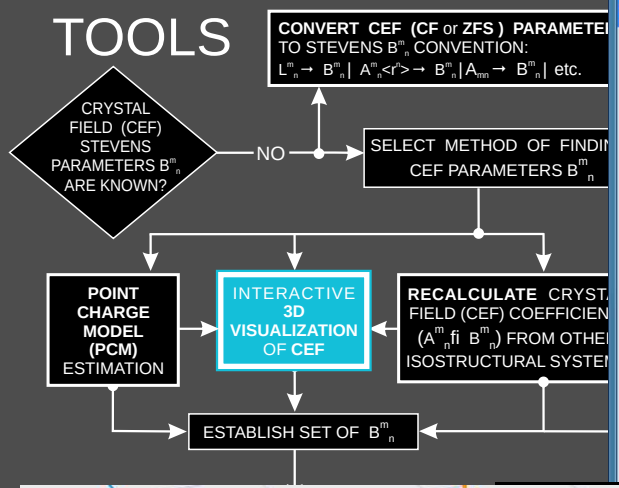


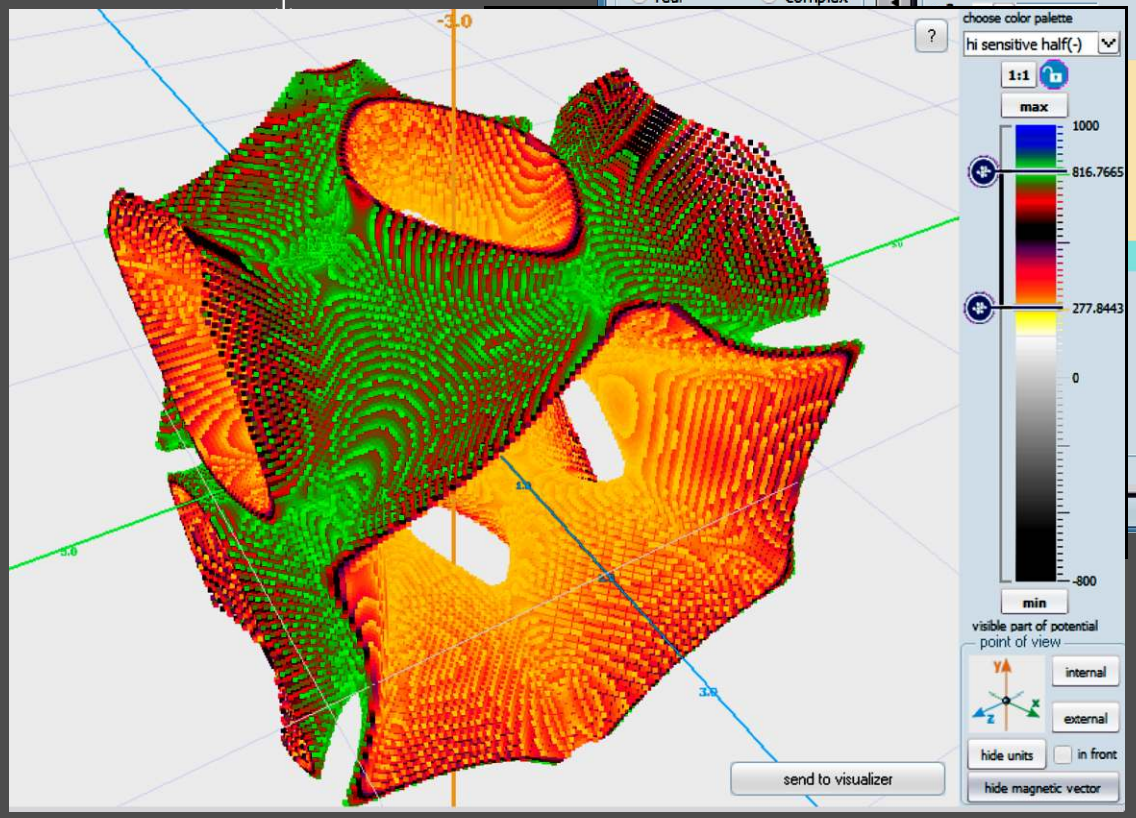
AVAILABLE PRIMITIVE POINT-CHARGE SYMMETRIES

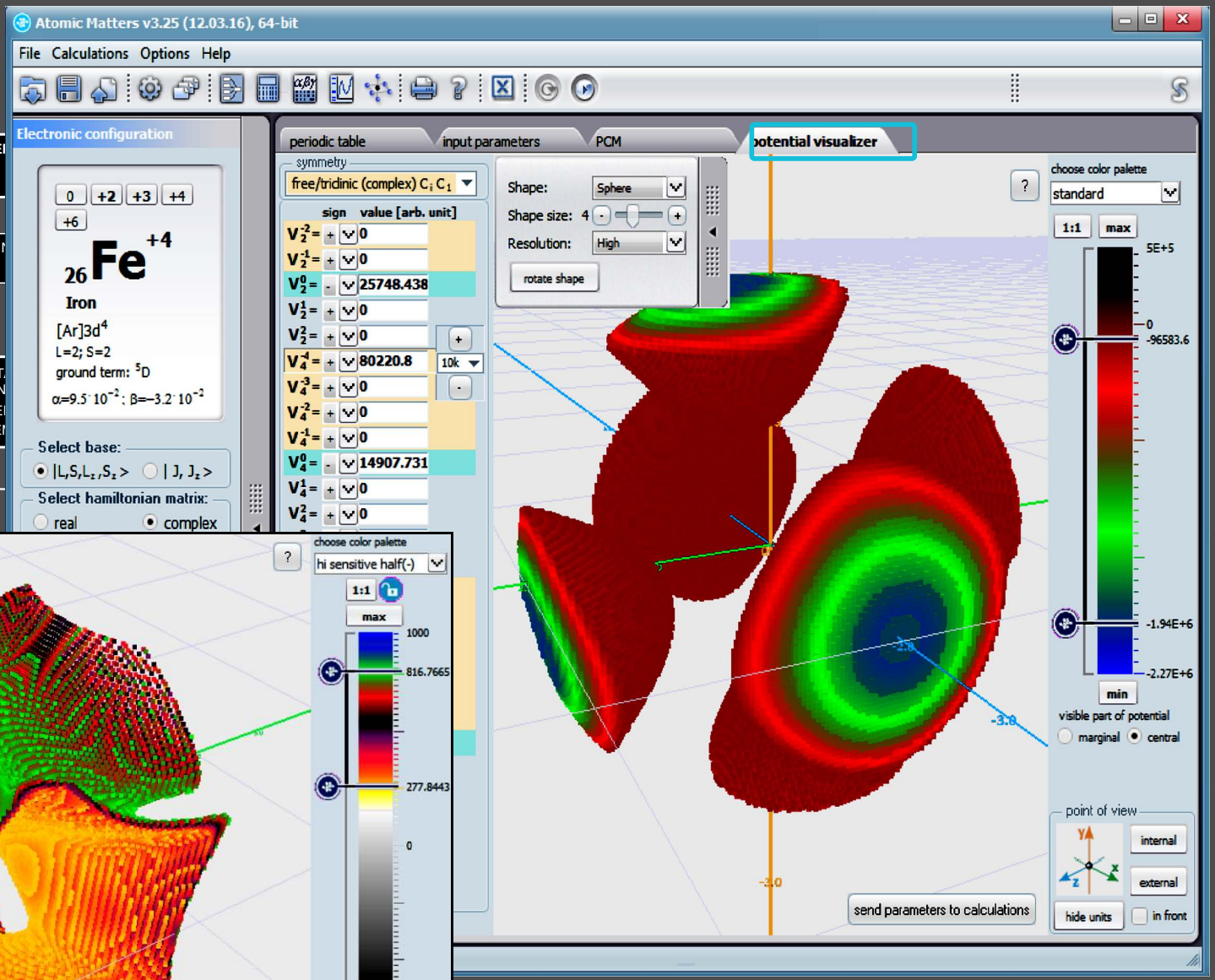


atomic matters CEF POTENTIALVISUALIZER 3D interactive tool

CEF POTENTIAL VISUALIZER ③

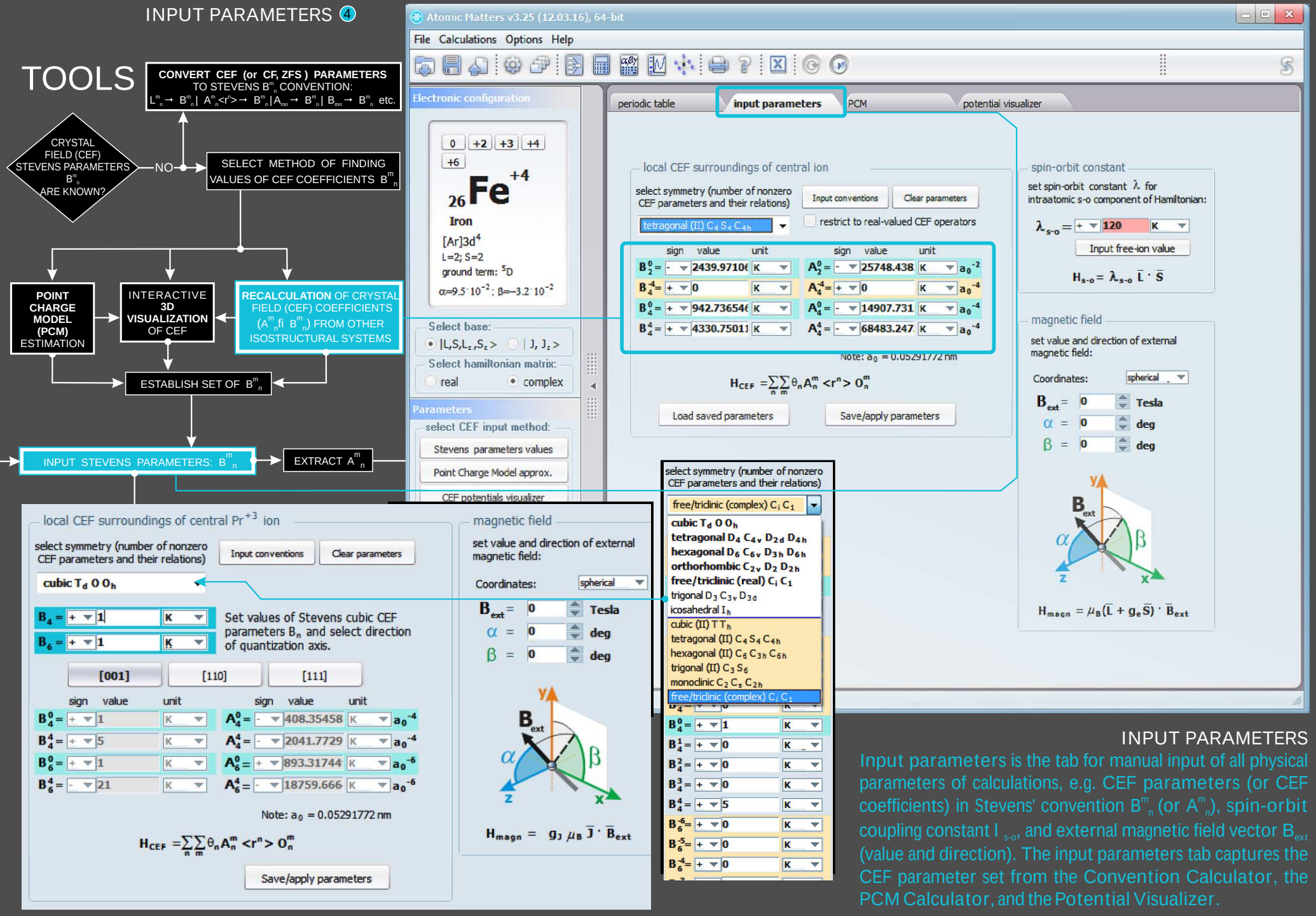






The Potential Visualizer offers a full 3D interactive (OpenGL graphics engine) view of potential defined by CEF coefficients. The user can change CEF coefficients smoothly, zoom, rotate, tilt, define borders and color palettes, and freely modify the CEF view in a Cartesian coordinate system. The Potential Visualizer is able to export CEF parameters to the Input Parameters tab with a defined scaling factor to simulate the shielding effect of an unclosed electron shell.

INPUT PARAMETERS ④



INPUT PARAMETERS

Input parameters is the tab for manual input of all physical parameters of calculations, e.g. CEF parameters (or CEF coefficients) in Stevens' convention B^m_n (or A^m_n), spin-orbit coupling constant l_{s-o}, and external magnetic field vector B_{ext} (value and direction). The input parameters tab captures the CEF parameter set from the Convention Calculator, the PCM Calculator, and the Potential Visualizer.

atomic matters CALCULATORS (Stevens Factors calculator, Units calculator, Convention calculator)

CALCULATORS 5

TOOLS

CRYSTAL FIELD **CEF** STEVENS PARAMETERS B^m_n ARE KNOWN?

NO

SELECT METHOD OF FINDING VALUES OF CEF COEFFICIENTS B^m_n

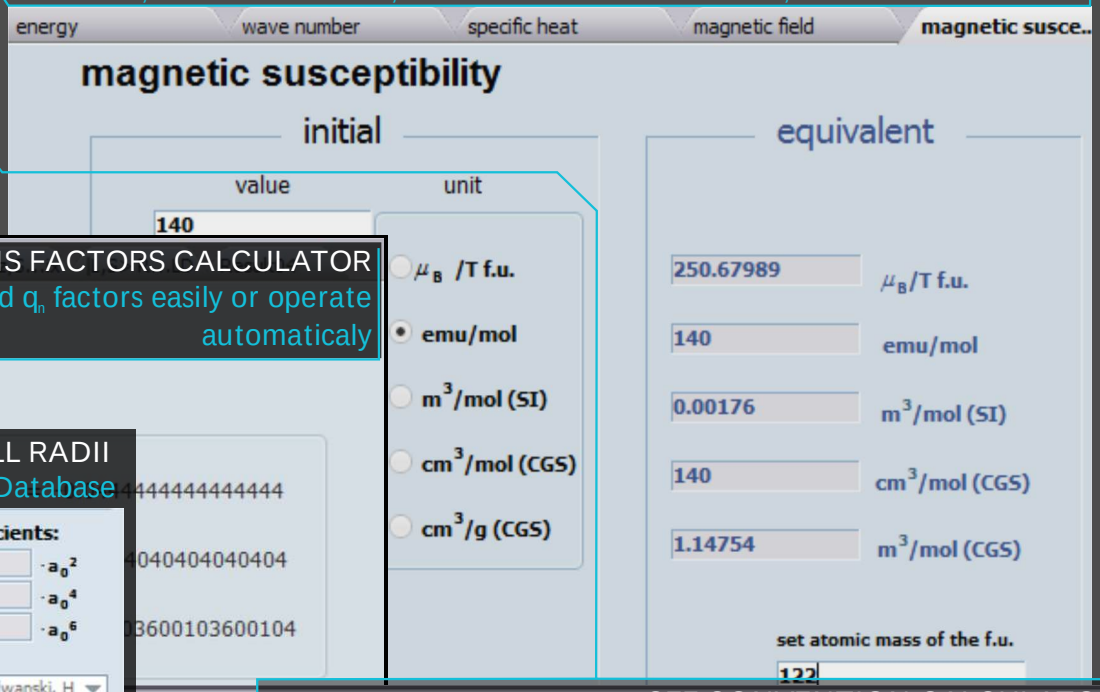
CONVERT CEF (CF or ZFS) PARAMETERS TO STEVENS B^m_n CONVENTION:
$L^m_n \rightarrow B^m_n$ | $A^m_n\langle r^n\rangle \rightarrow B^m_n$ | $A_{mn} \rightarrow B^m_n$ | etc.

POINT CHARGE MODEL (PCM) ESTIMATION

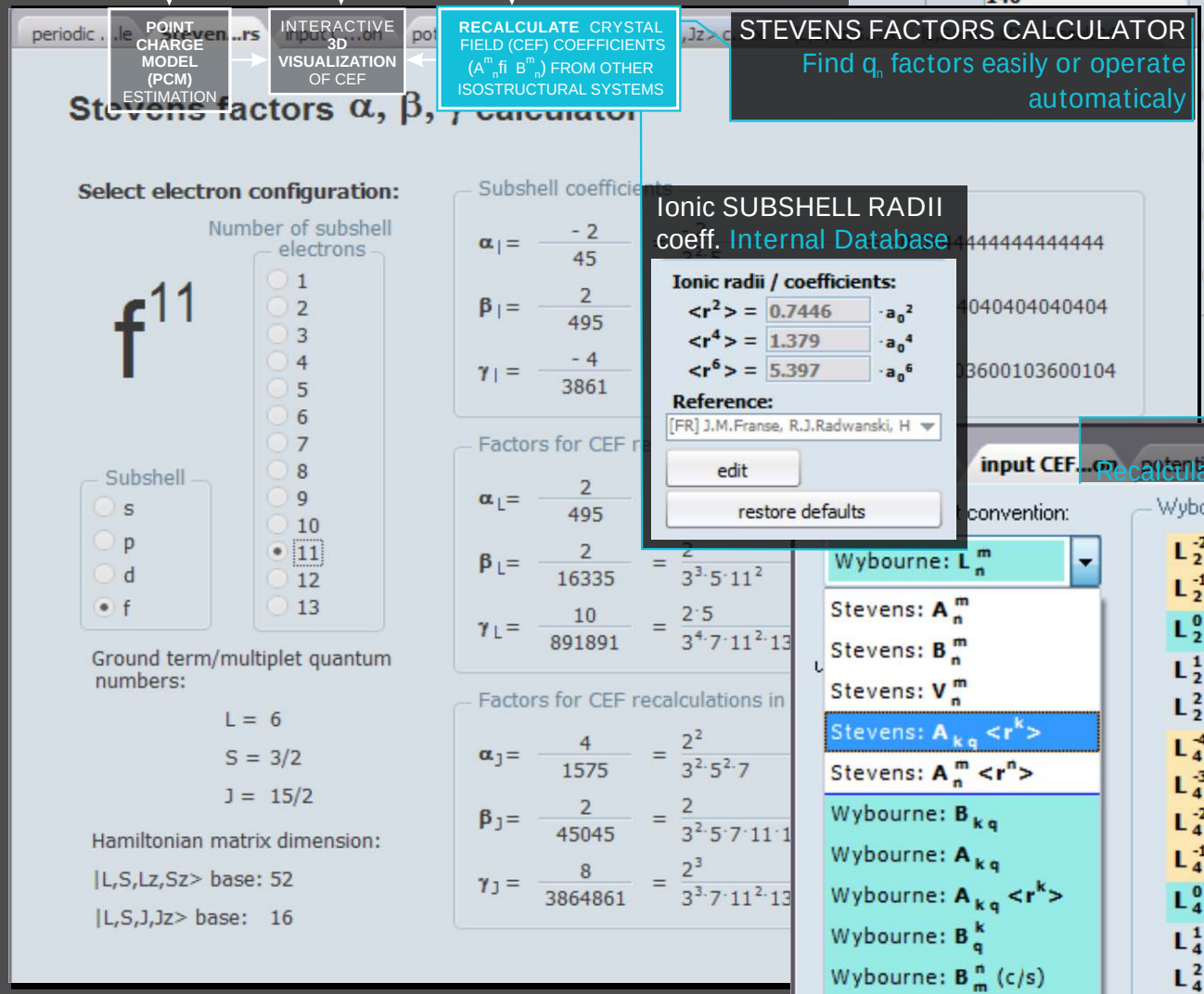
INTERACTIVE **3D VISUALIZATION** OF CEF

RECALCULATE CRYSTAL FIELD (CEF) COEFFICIENTS (A^m_nfi B^m_n) FROM OTHER ISOSTRUCTURAL SYSTEMS

UNITS CALCULATOR
Easily recalculate units of: ATOMIC SCALE ENERGY, WAVE NUMBER, MAGNETIC FIELD, MAGNETIC SUSCEPTIBILITY, SPECIFIC HEAT ...

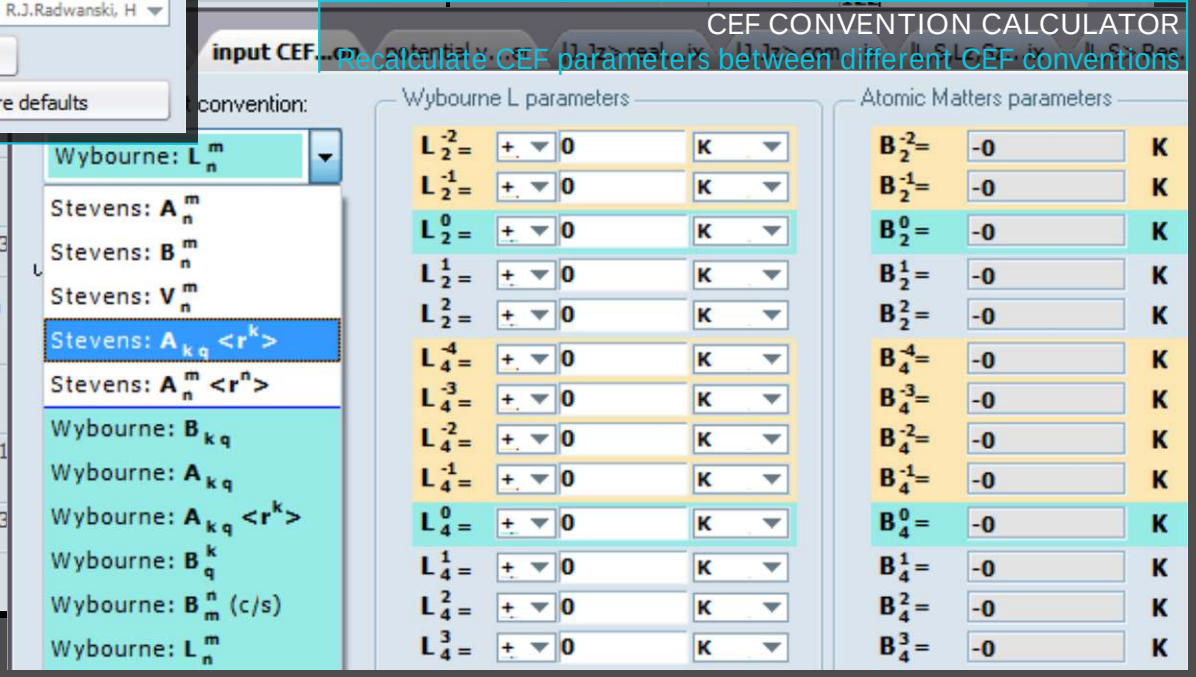


STEVENS FACTORS CALCULATOR
Find q_n factors easily or operate automaticaly



Ionic SUBSHELL RADII coeff. Internal Database

CEF CONVENTION CALCULATOR
Recalculate CEF parameters between different CEF conventions

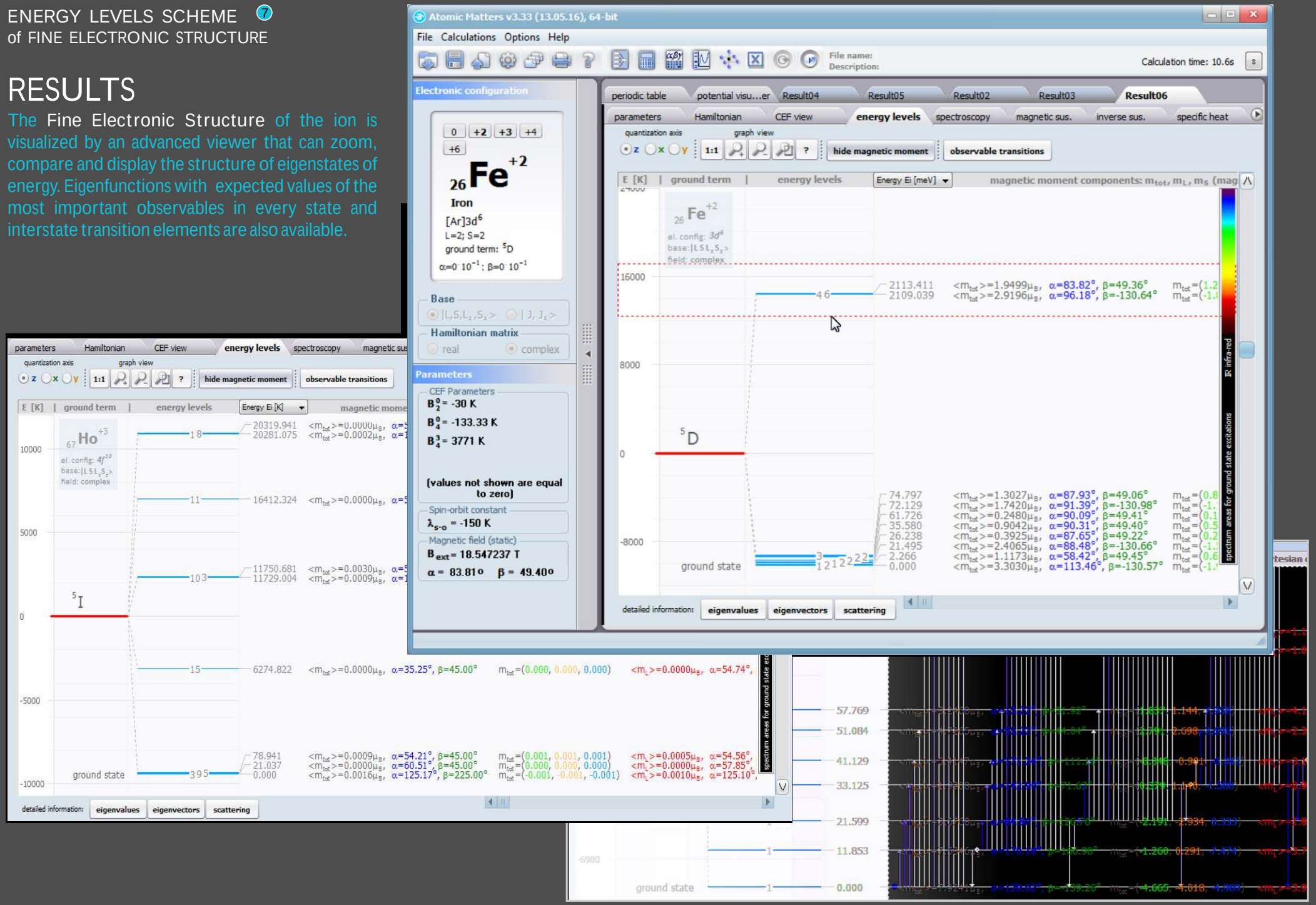


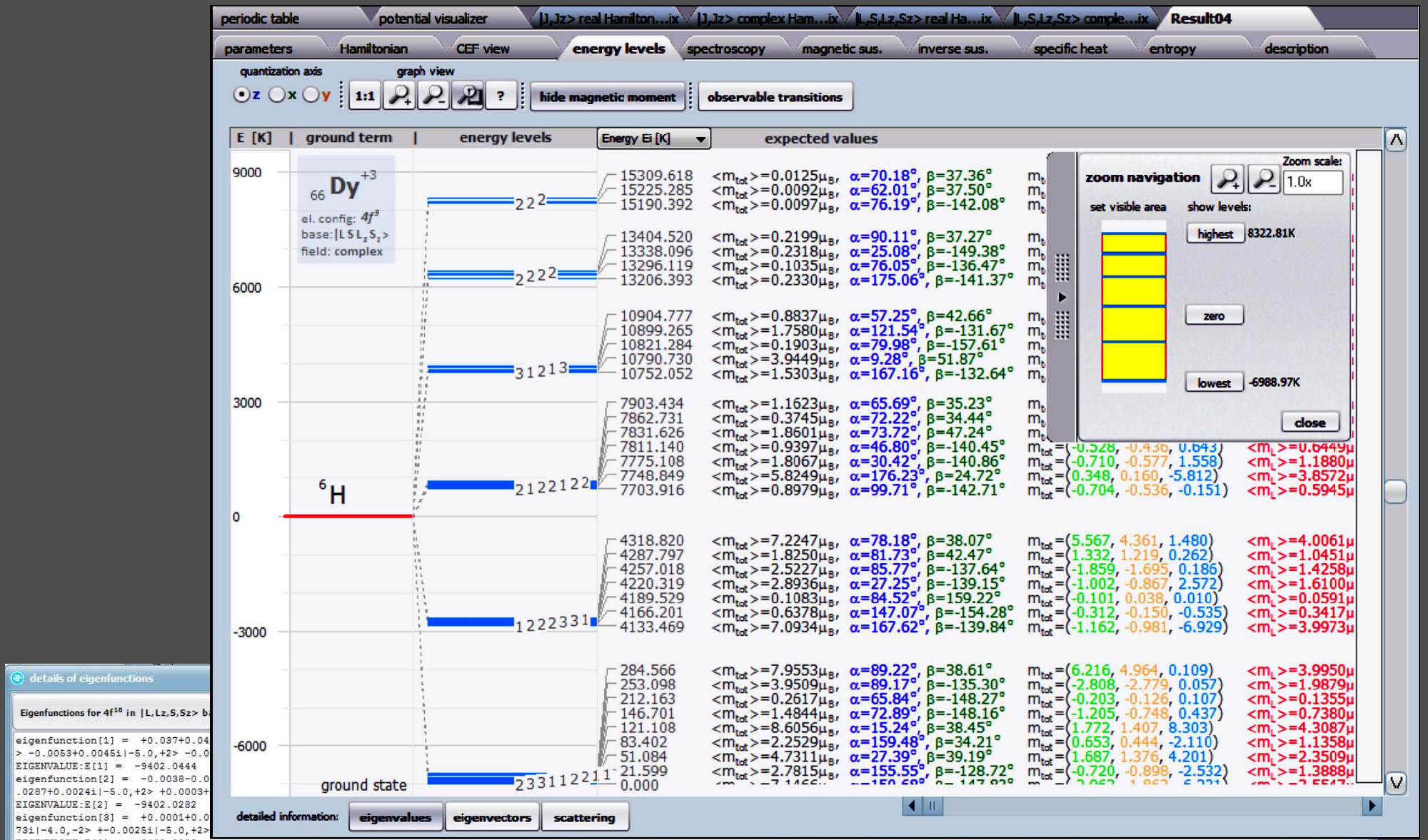
The Hamiltomian matrix elements view is always available on a dedicated sub-tab containing discrete matrix elements created by Crystal Electric Field (CEF) interactions, intra-atomic spin-orbit interactions (Russel-Saunders coupling), and external magnetic field interactions (Zeeman effect).
This tab offers independent verification of calculations and, due to the explicit form, performs an educational function as it displays how operators generate matrix elements according to electromagnetic interactions defined by the chosen Hamiltonian.

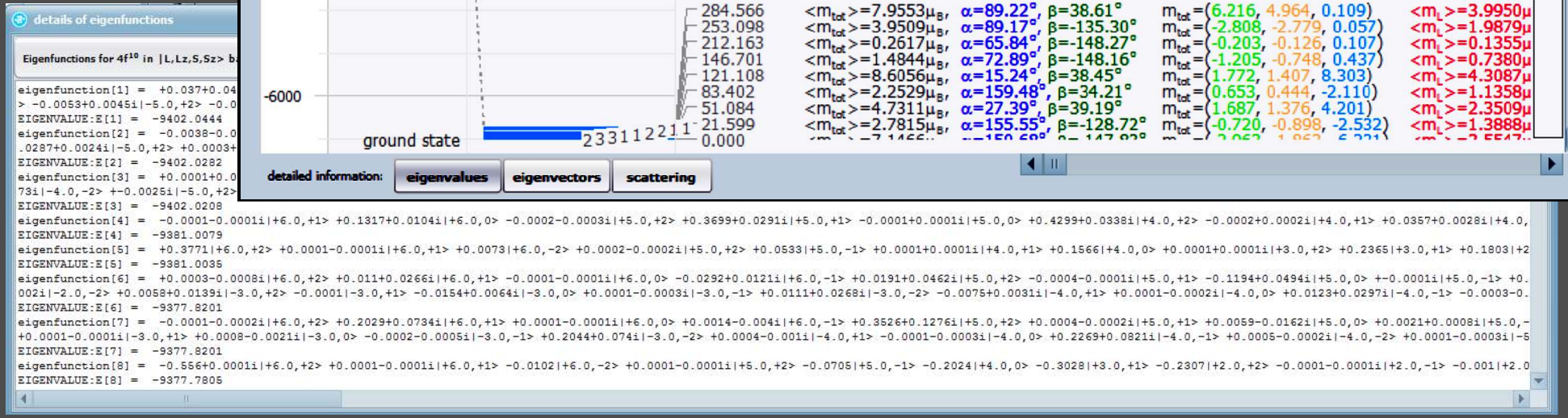
ENERGY LEVELS SCHEME ⑦
of FINE ELECTRONIC STRUCTURE

RESULTS

The Fine Electronic Structure of the ion is visualized by an advanced viewer that can zoom, compare and display the structure of eigenstates of energy. Eigenfunctions with expected values of the most important observables in every state and interstate transition elements are also available.



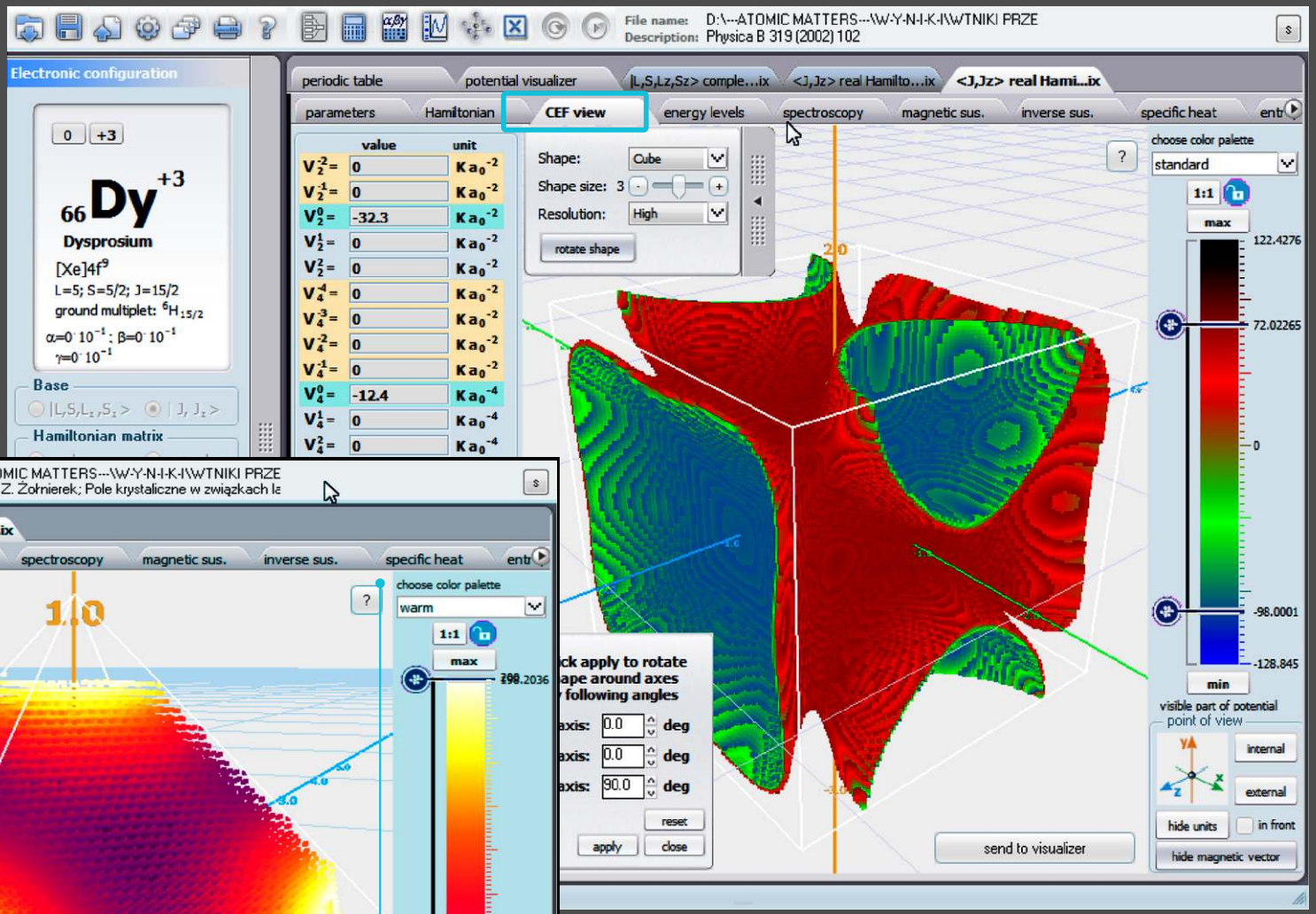

periodic table
potential visualizer
|J,Jz> real Hamilton...ix
|J,Jz> complex Ham...ix
|L,S,Lz,Sz> real Ha...ix
|L,S,Lz,Sz> comple...ix
Result04
parameters
Hamiltonian
CEF view
energy levels
spectroscopy
magnetic sus.
inverse sus.
specific heat
entropy
description
quantization axis
z x y
graph view
1:1
?
hide magnetic moment
observable transitions
E [K]
ground term
energy levels
Energy Ei [K]
expected values
66 Dy +3
el. config: 4f9
base:|L S Lz Sz>
field: complex
6 H
ground state
zoom navigation
Zoom scale:
1.0x
set visible area
show levels:
highest
8322.81K
zero
lowest
-6988.97K
close
detailed information:
eigenvalues
eigenvectors
scattering


details of eigenfunctions
Eigenfunctions for 4f10 in |L,Lz,S,Sz> b
EIGENVALUE:E[1] = -9402.0444
EIGENVALUE:E[2] = -9402.0282
EIGENVALUE:E[3] = -9402.0208
EIGENVALUE:E[4] = -9381.0079
EIGENVALUE:E[5] = -9381.0035
EIGENVALUE:E[6] = -9377.8201
EIGENVALUE:E[7] = -9377.8201
EIGENVALUE:E[8] = -9377.7805

CEF VIEW ⑧
CEF POTENTIAL VISUALIZATION

RESULTS

CEF view is a sub-tab of result tabs and has similar functionality to the Potential Visualizer in the TOOLS section but without interactive CEF design. The CEF view sub-tab only shows potential defined by CEF parameters for a whole set of results in a result tab. The user can zoom, rotate, tilt, define borders and color palettes, and freely modify the view.



RESULTS

NEW SET OF RESULS FOR SELECTED ATOM/ION IN CEF ENVIRONMENT

- 3-Dimensional, interactive visualization of CEF, extracted CEF coefficients A^m_n
- Fine electronic structure of ions, Spectrum simulations and all calculation settings
- Directional components (x,y,z) or (x,z) of magnetic properties of ions
- Temperature dependencies of electronic, magnetic and thermodynamic properties of material are contained in chosen ions in defined crystal surrounding

INTERACTIVE VISUALISATIONS

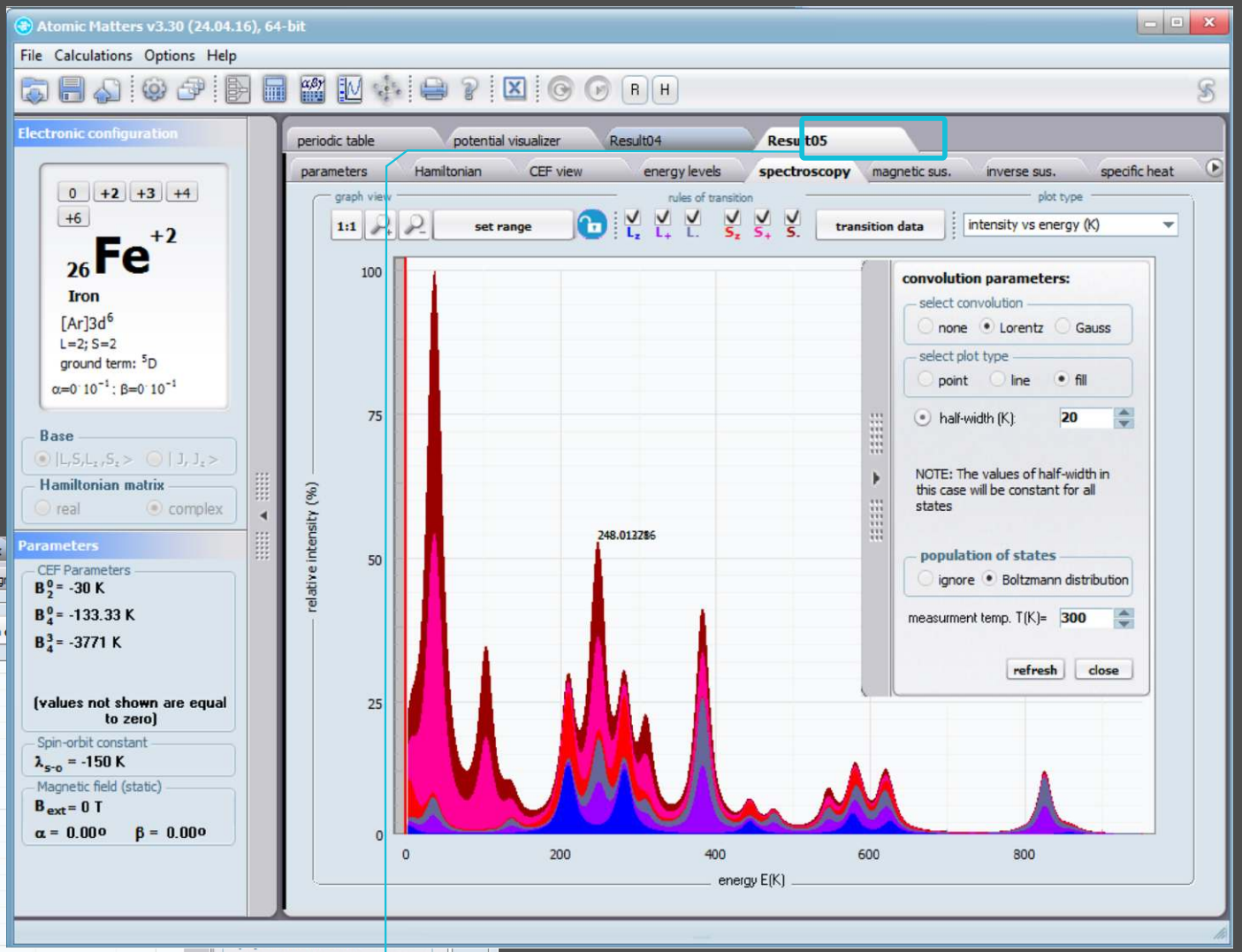
RESULT DATA COMPARISON TOOLS (**MCE**)

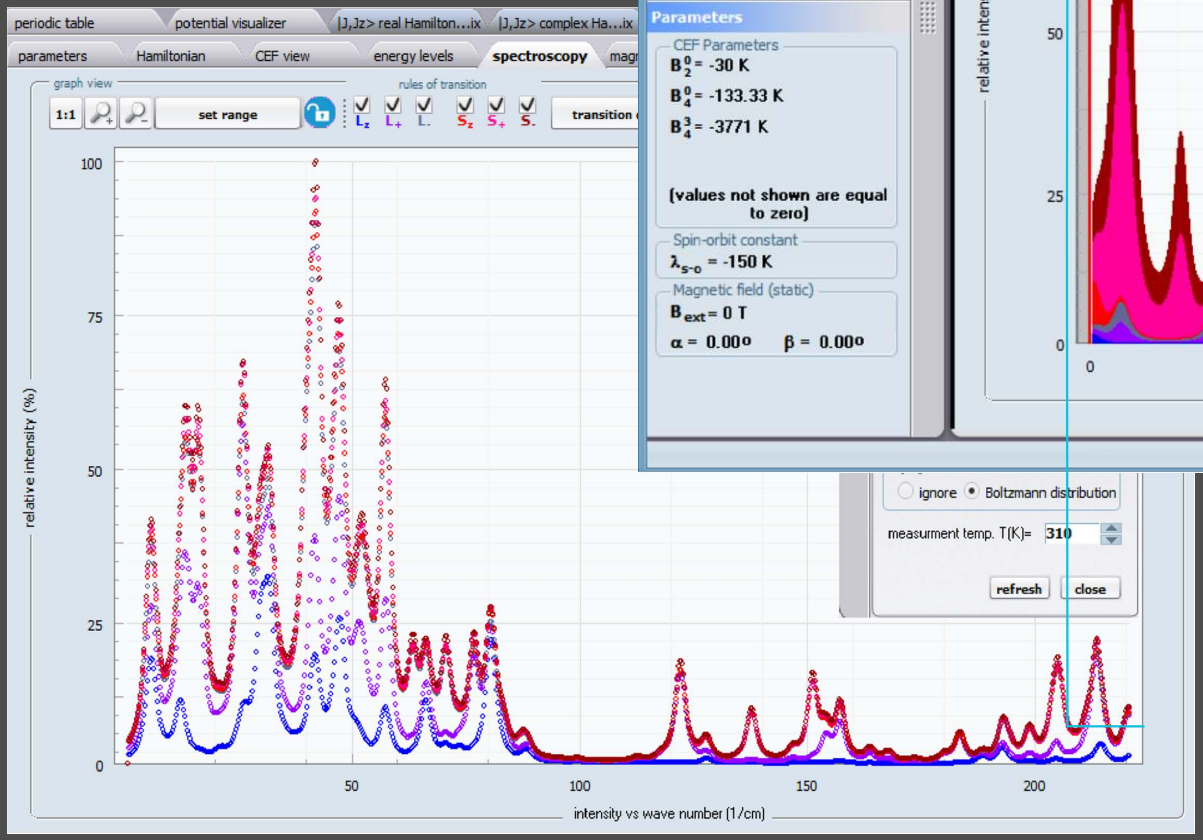
EXPORT DATA

STORE in ***.atma** FILE

RESULTS

The absorption spectrum of calculated Fine Electronic Structure can be simulated with different spectroscopy methods, temperatures, and resolutions. Analyzed area of spectrum and visibility of spectrum components can be adjusted. Spectra from different sets of results can be easily compared by zooming and locking comparable areas. Units and plots can be selected to compare results with published experimental data.





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INTERACTIVE VISUALISATIONS

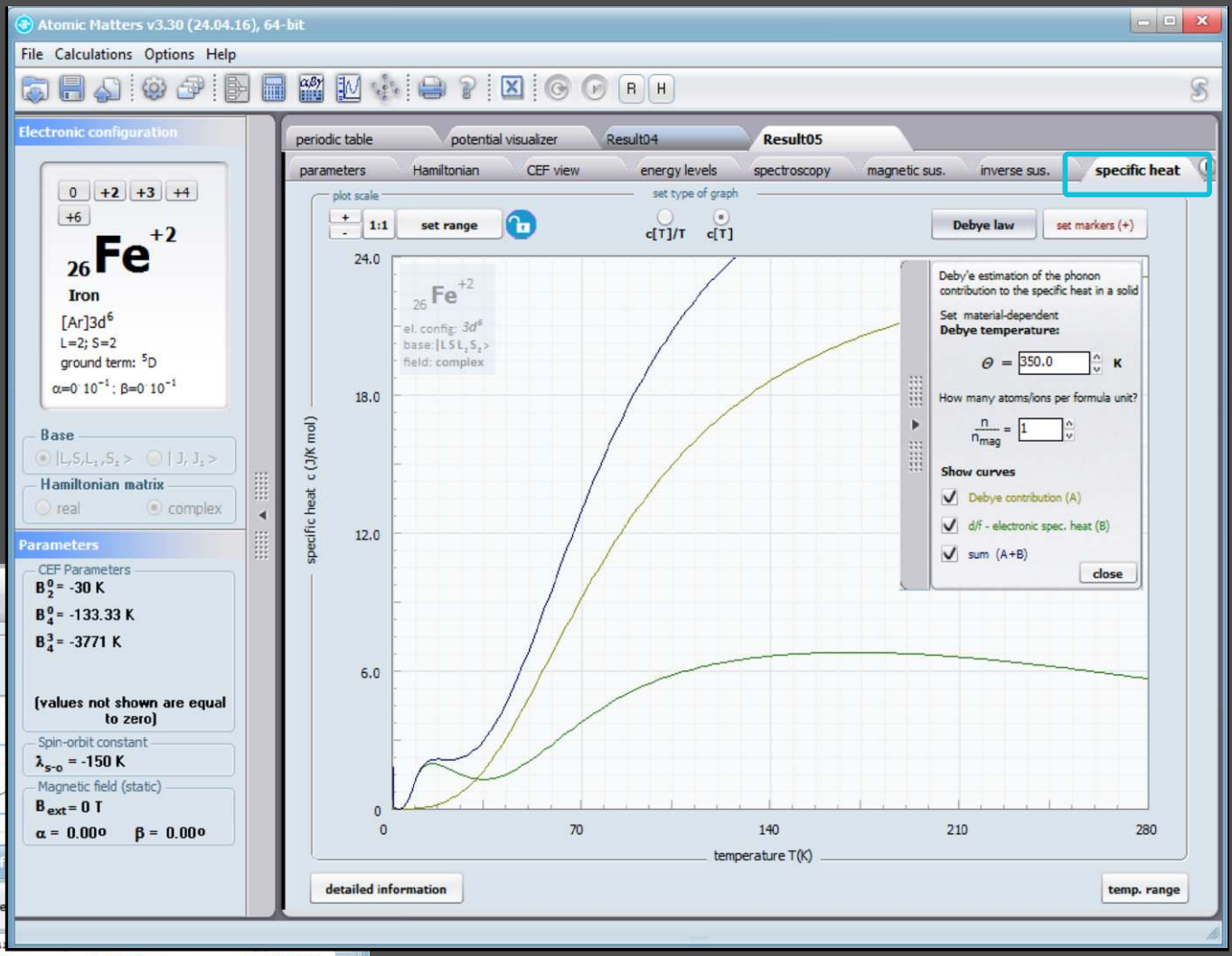
RESULT DATA COMPARISON TOOLS (**MCE**)

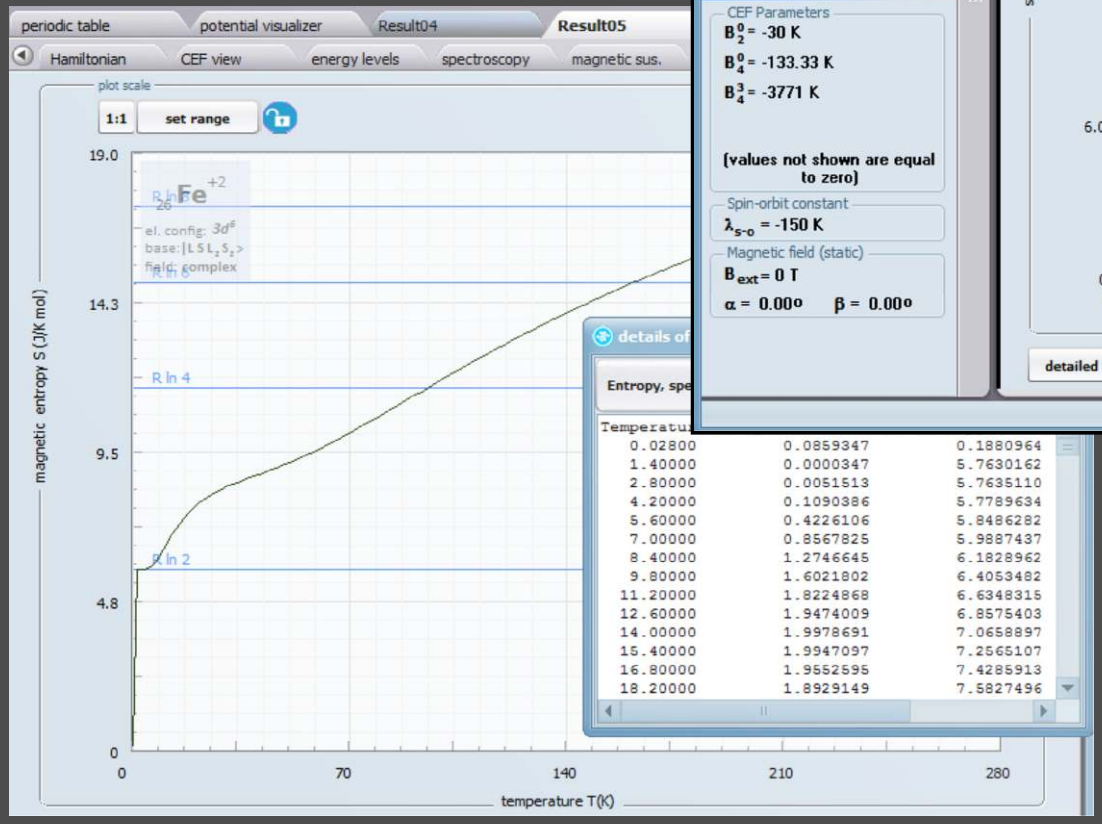
EXPORT DATA

STORE in ***.atma** FILE

RESULTS

Visualizations of thermal evolution of molar specific heat of a localized electron system (Schottky specific heat contribution) and thermal variation of entropy of such an electron system (magnetic entropy) are displayed on unified interactive graphs. Additionally, the interactive graph of specific heat can simulate a crystal lattice contribution to full specific heat (Debye specific heat). The plot of magnetic entropy displays comparable values of statistical entropy and is useful for Magnetocaloric Effect (MCE) estimations. All graphs can be freely resized in 2 dimensions and filled manually with additional points (experimental, reference data).





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INTERACTIVE VISUALISATIONS

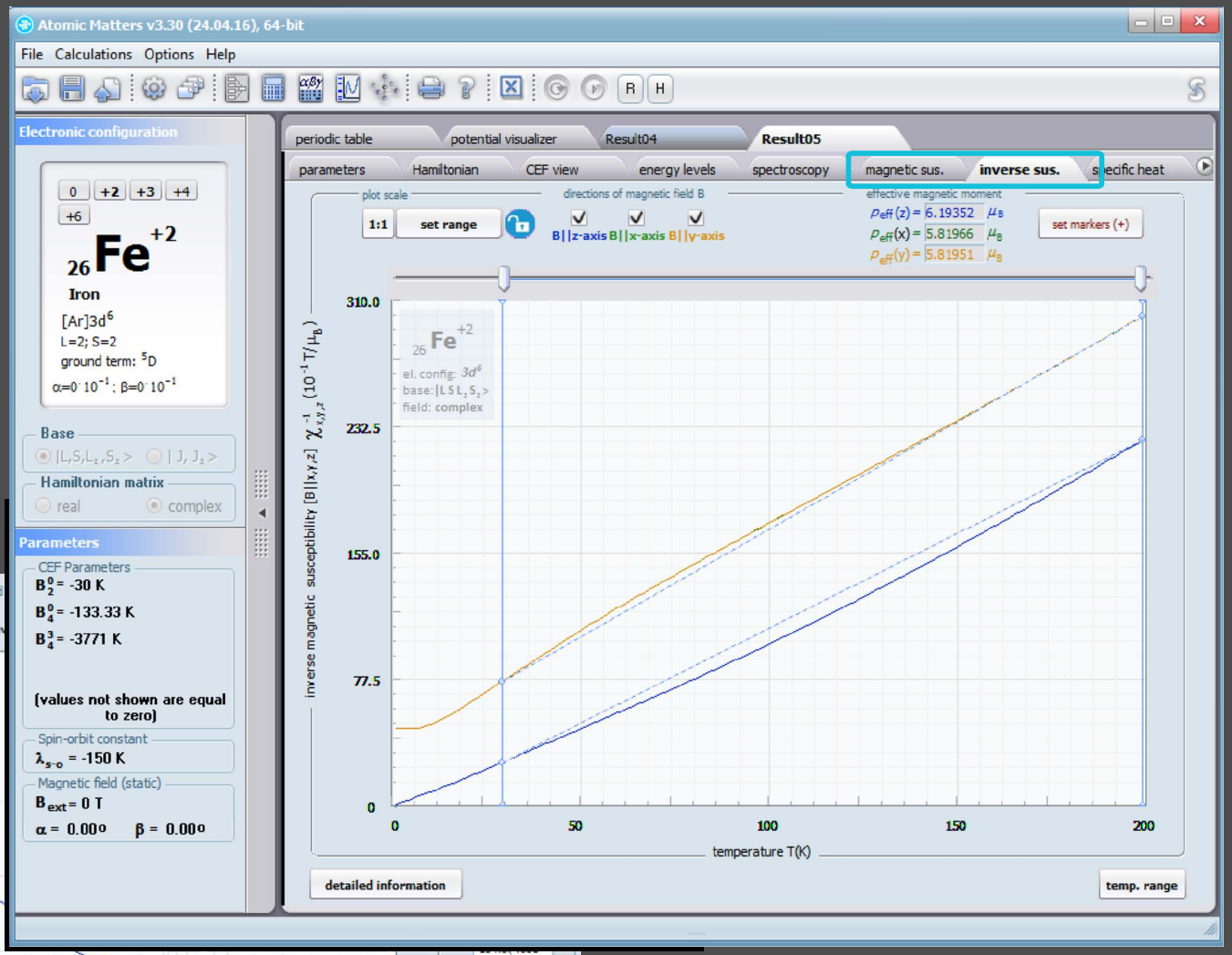
RESULT DATA COMPARISON TOOLS (**MCE**)

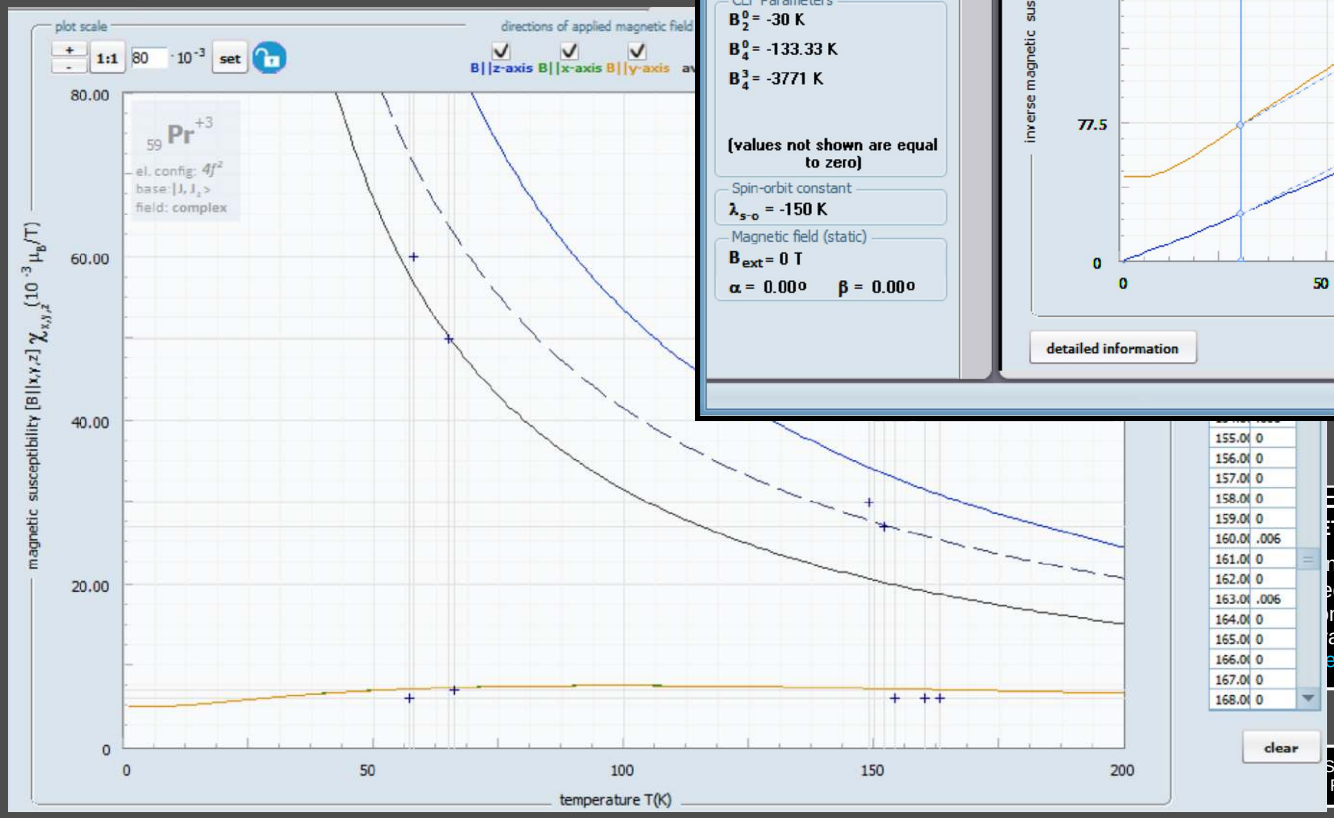
EXPORT DATA

ARCHIVISATION ***.atma** FILE

RESULTS

2 graphs of thermal variation of magnetic susceptibility for orthogonal directions of an inducing magnetic field are shown. Obtained temperature variations of magnetic susceptibility can be compared with interactive Curie Low curves plotted for a given effective magnetic moment. Susceptibility plots can be calculated both for established value and direction of external magnetic field (for ordered state simulation) as well as without an established external field, under the influence of 'zero field' set up in 'Preferences'.
Susceptibility graphs can be filled by additional points (experimental data) and can be freely zoomed and edited.





RESULTS

T OF RESULS FOR SELECTED ATOM/ION IN CEF ENVIRONMENT

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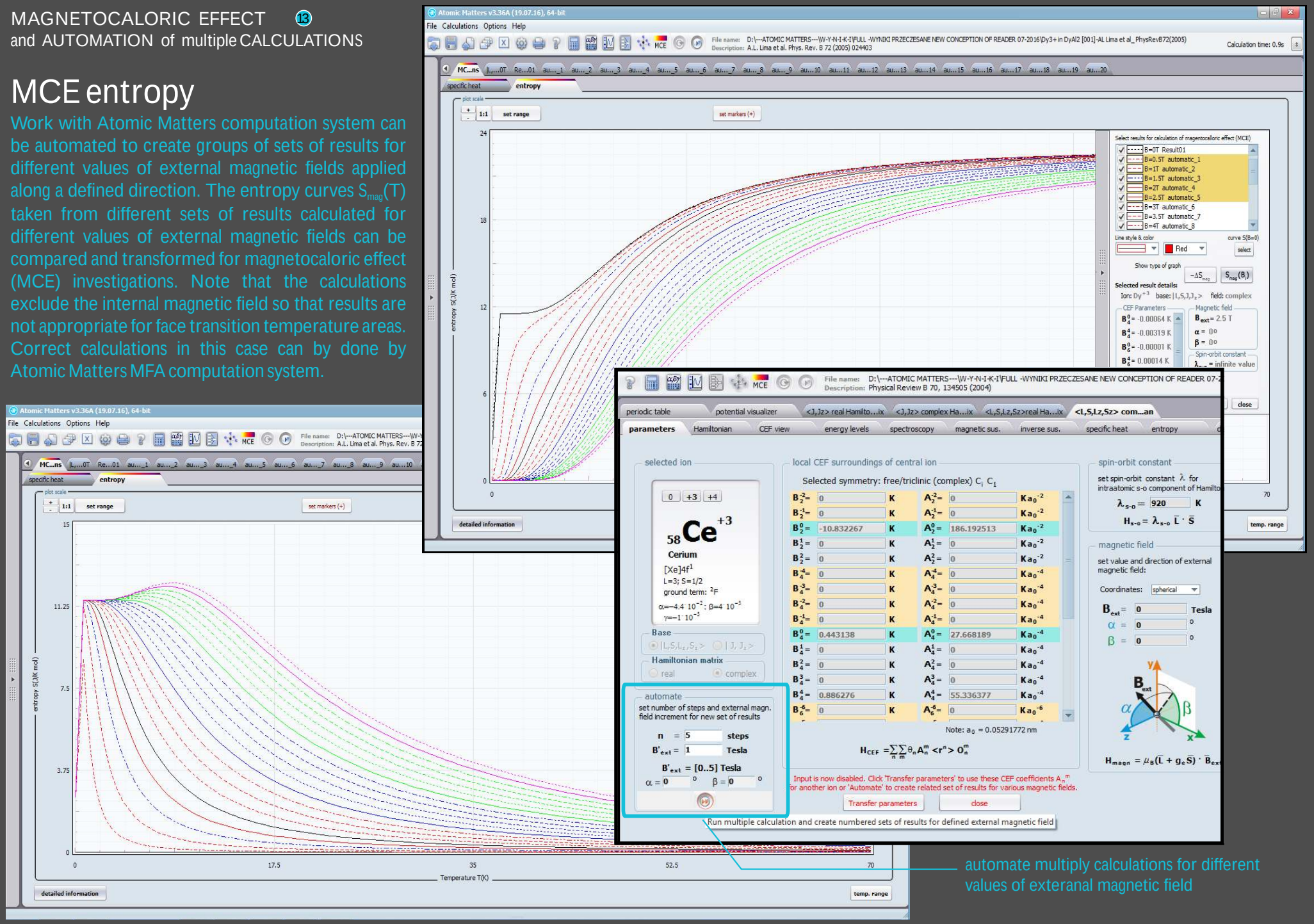
ctronic structure of ions, Spectrum simulations and all calculation settings
nal components (x,y,z) or (x,z) of magnetic properties of ions
ature dependencies of electronic, magnetic and thermodynamic properties
erial are contained in chosen ions in defined crystal surrounding

SATION FILE
RESULT DATA COMPARISON TOOLS (**MCE**)
EXPORT DATA
INTERACTIVE VISUALISATIONS

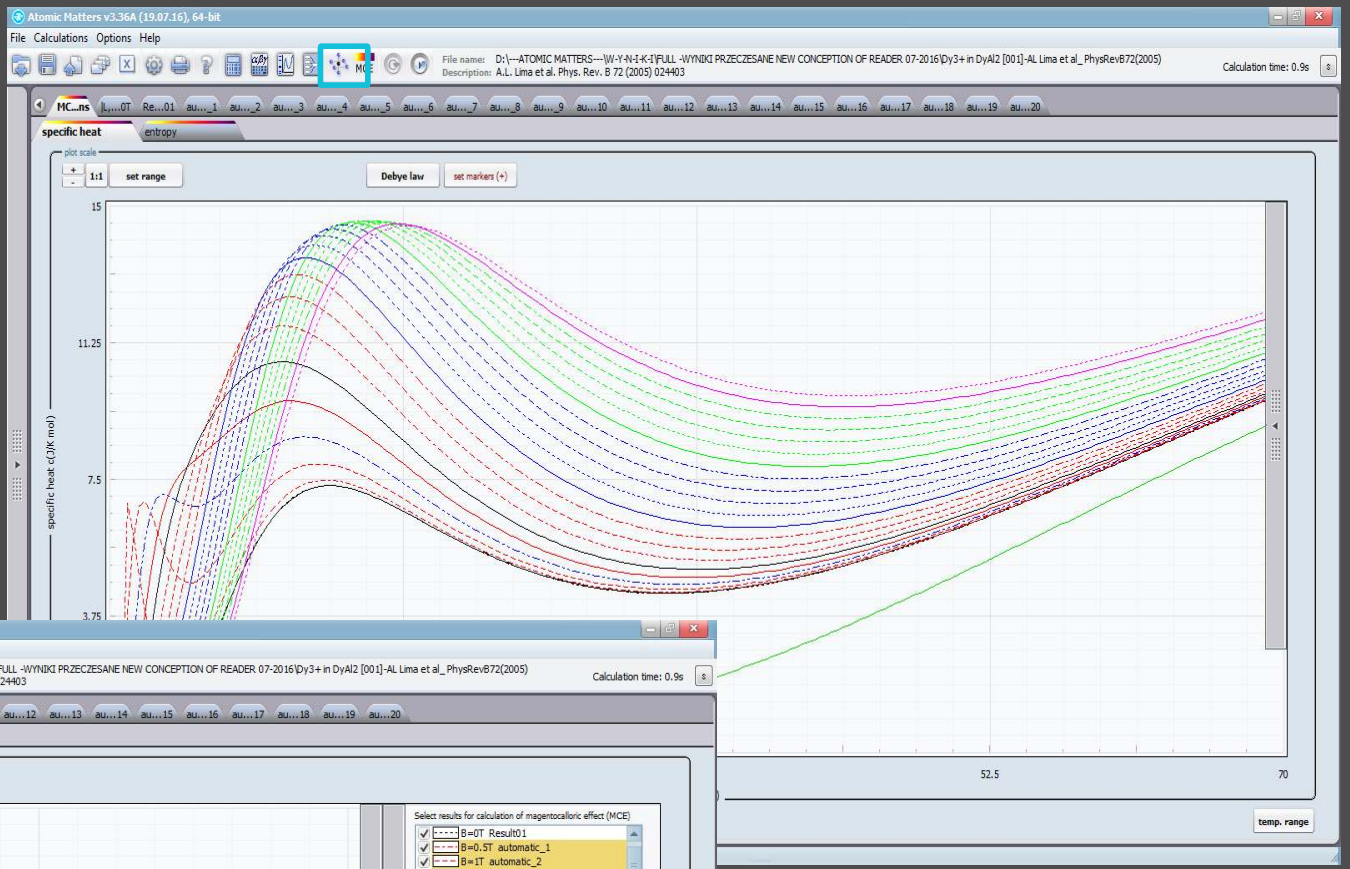
MCE entropy

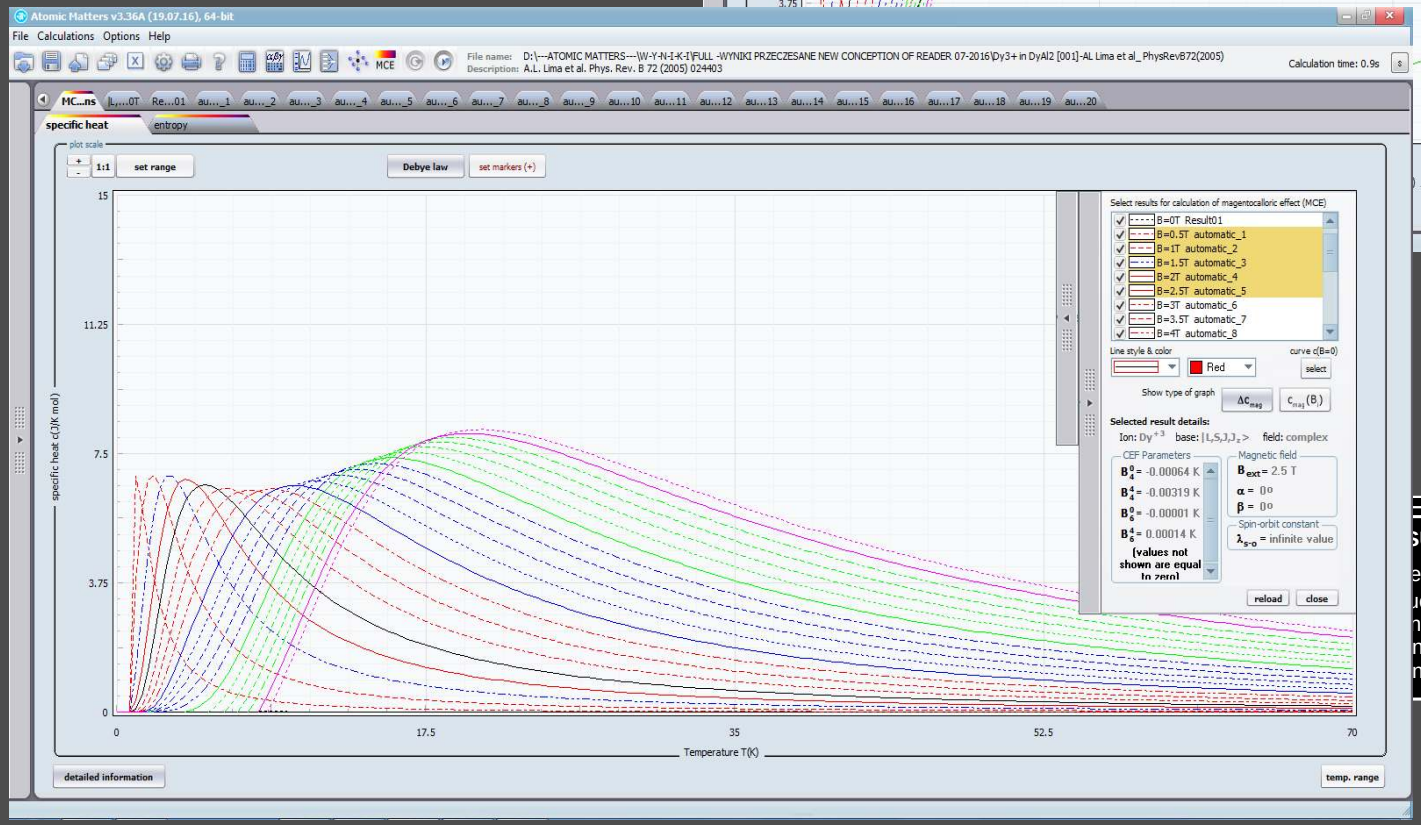
Work with Atomic Matters computation system can be automated to create groups of sets of results for different values of external magnetic fields applied along a defined direction. The entropy curves $S_{mag}(T)$ taken from different sets of results calculated for different values of external magnetic fields can be compared and transformed for magnetocaloric effect (MCE) investigations. Note that the calculations exclude the internal magnetic field so that results are not appropriate for face transition temperature areas. Correct calculations in this case can by done by Atomic Matters MFA computation system.



MCE specific heat

The electronic specific heat curves c(T) (with Debye' crystal lattice component) taken from different sets of results calculated for different values of external magnetic fields can be compared and transformed on MCE sub-tab for magnetocaloric effect (MCE) investigations. The user-frendly interface allows curves to be added, removed, and transformed according to MCE (magnetocaloric effect) investigations for stable thermodynamic regions. Note that the calculations exclude the internal magnetic field so that results are not appropriate for face transition temperature areas. Correct calculations in this case can by done by Atomic Matters MFA computation system.





RESULTS

SULS FOR SELECTED ATOM/ION IN CEF ENVIRONMENT

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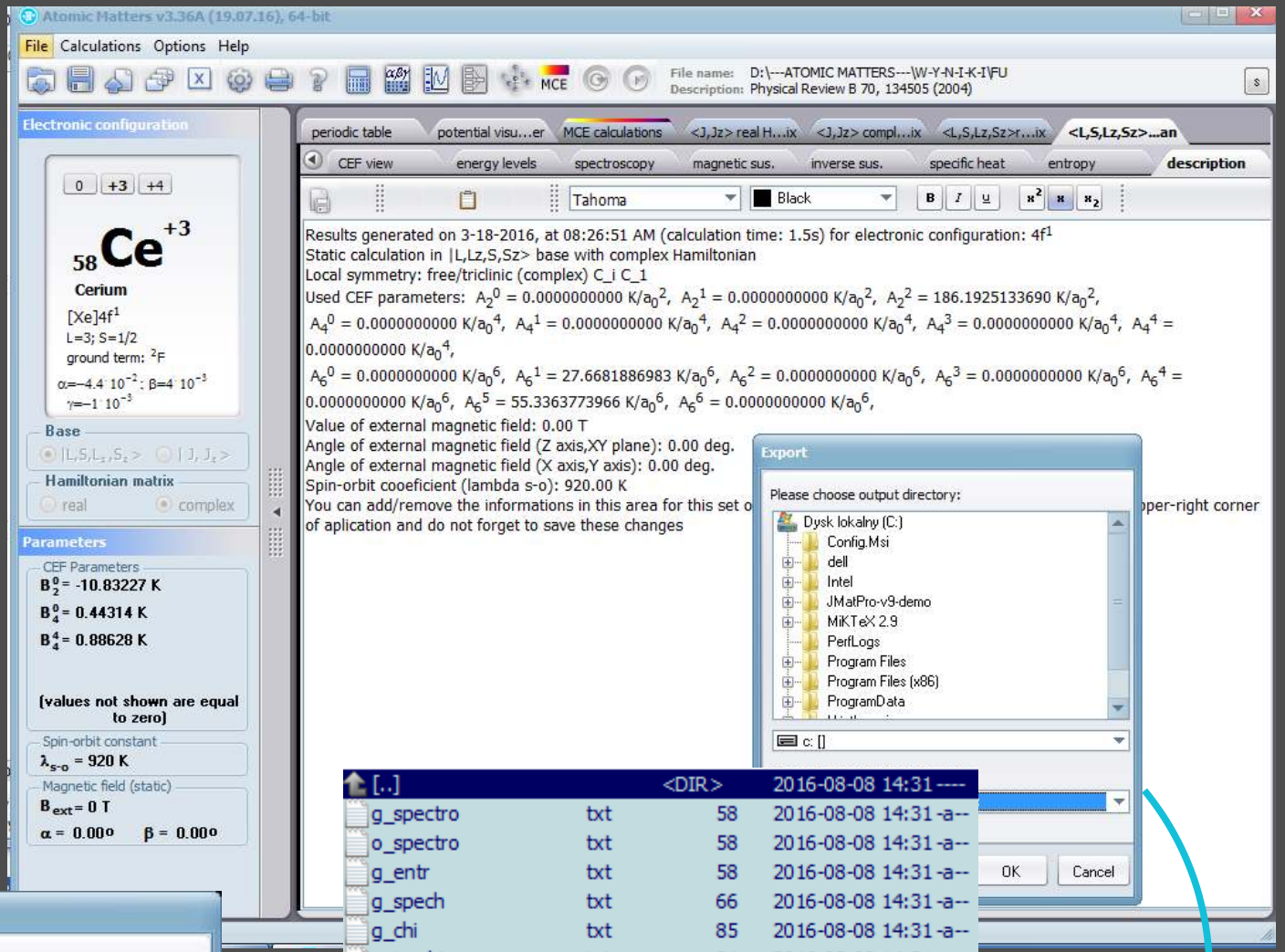
nents (x,y,z) or (x,z) of magnetic properties of ions
ndencies of electronic, magnetic and thermodynamic properties
ntained in chosen ions in defined crystal surrounding

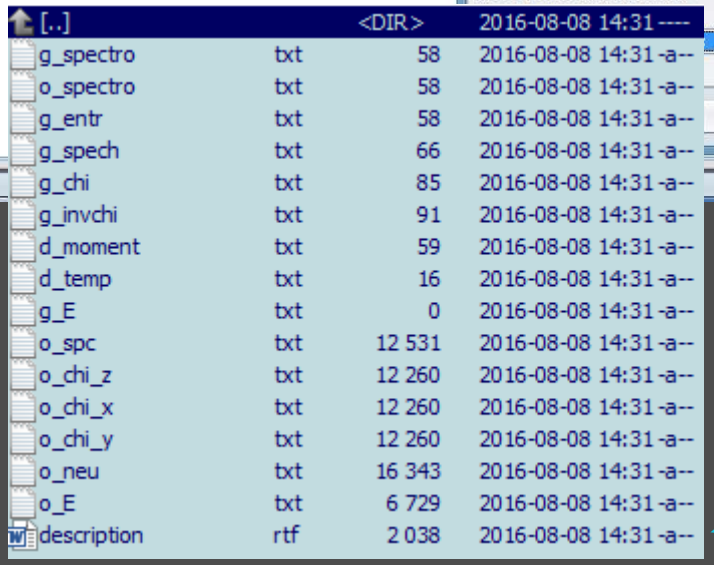
- INTERACTIVE VISUALISATIONS
- EXPORT DATA
- RESULT DATA COMPARISON TOOLS (**MCE**)

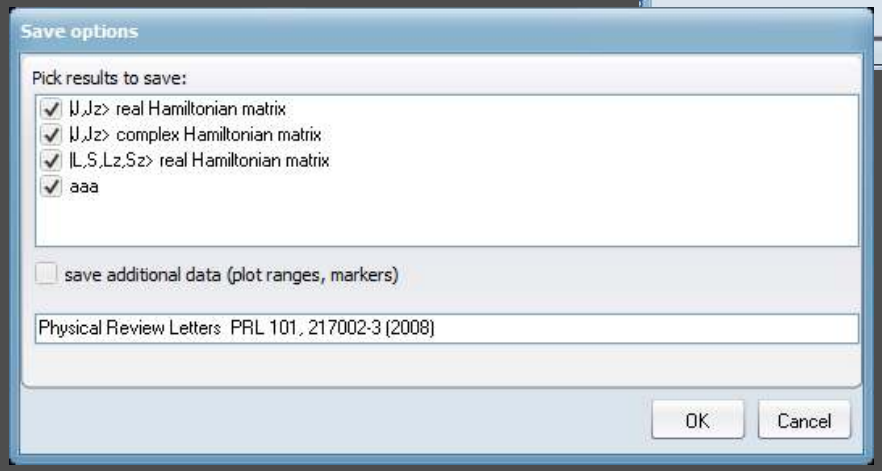
EXPORT and STORE result data ⑫

The output set generated by ATOMIC MATTERS system is visualized in a set of grouped tabs, available through a higher-order tab with the default name 'Resultxx' (where xx represents the number of the set of output files). Results may be exported or saved as text files. A set of output data is automatically supplemented by an information file containing the input data. This file is generated automatically at the start of the calculation (the round button 'Start Calculations') and contains information about the computed configuration, database, the method of calculation, the entered CEF coefficients, the value of $\lambda_{s\text{-}o}$ and the directional components of the magnetic field introduced into the calculation. Text information about the calculations can be supplemented manually with a simple text editor activated by clicking the desired output tab in the main window. The editing window can contain a convenient form of any text in the form of comments, requests, etc. and can be easily exported as text or *.rtf files.

All result information can be stored in unique *.atma files which contain whole sets of results in a special format that is readable by all programs in the ATOMIC MATTERS family.





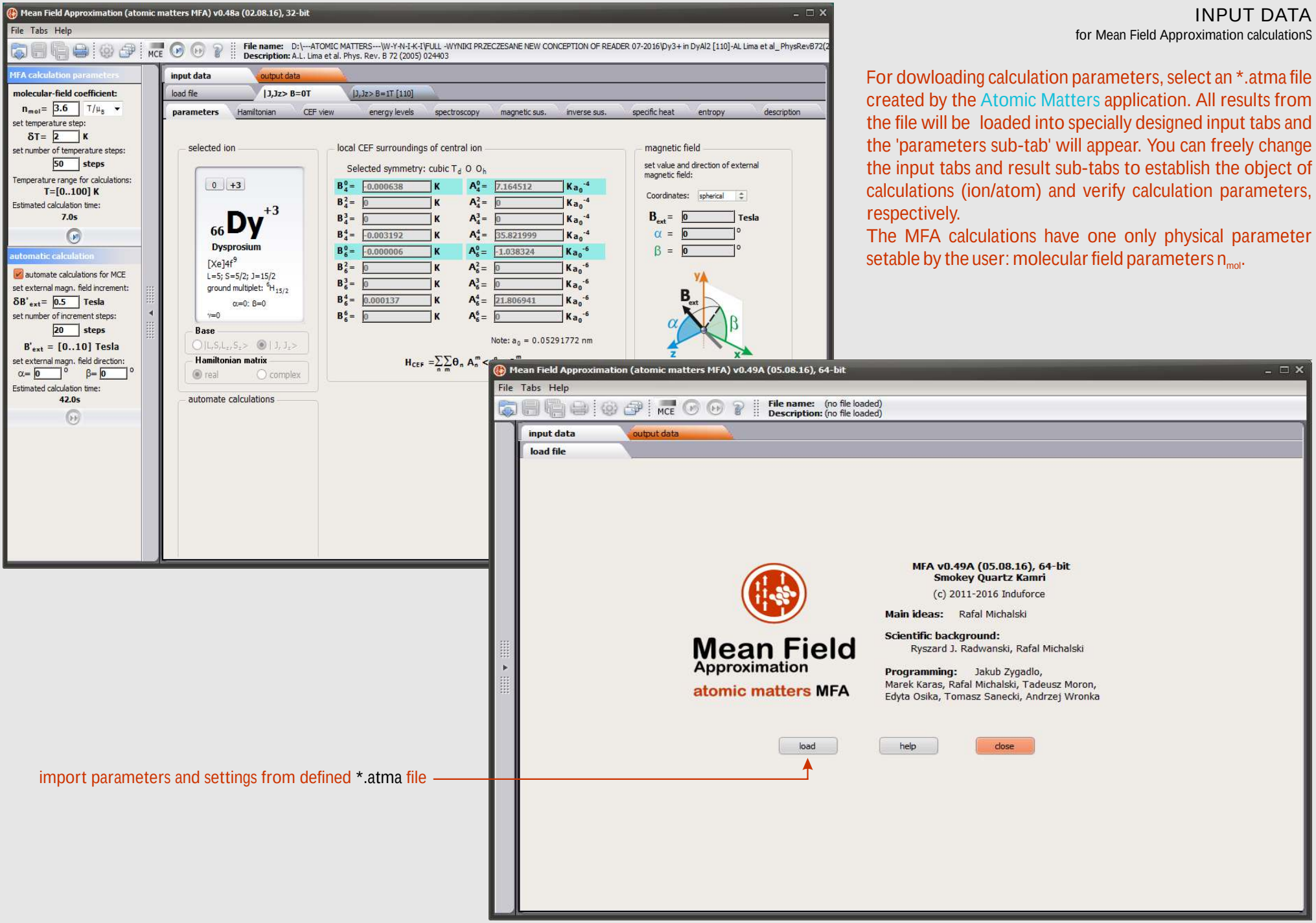


INPUT DATA

for Mean Field Approximation calculationS

For dowloading calculation parameters, select an *.atma file created by the Atomic Matters application. All results from the file will be loaded into specially designed input tabs and the 'parameters sub-tab' will appear. You can freely change the input tabs and result sub-tabs to establish the object of calculations (ion/atom) and verify calculation parameters, respectively.

The MFA calculations have one only physical parameter setable by the user: molecular field parameters n_{mol}.

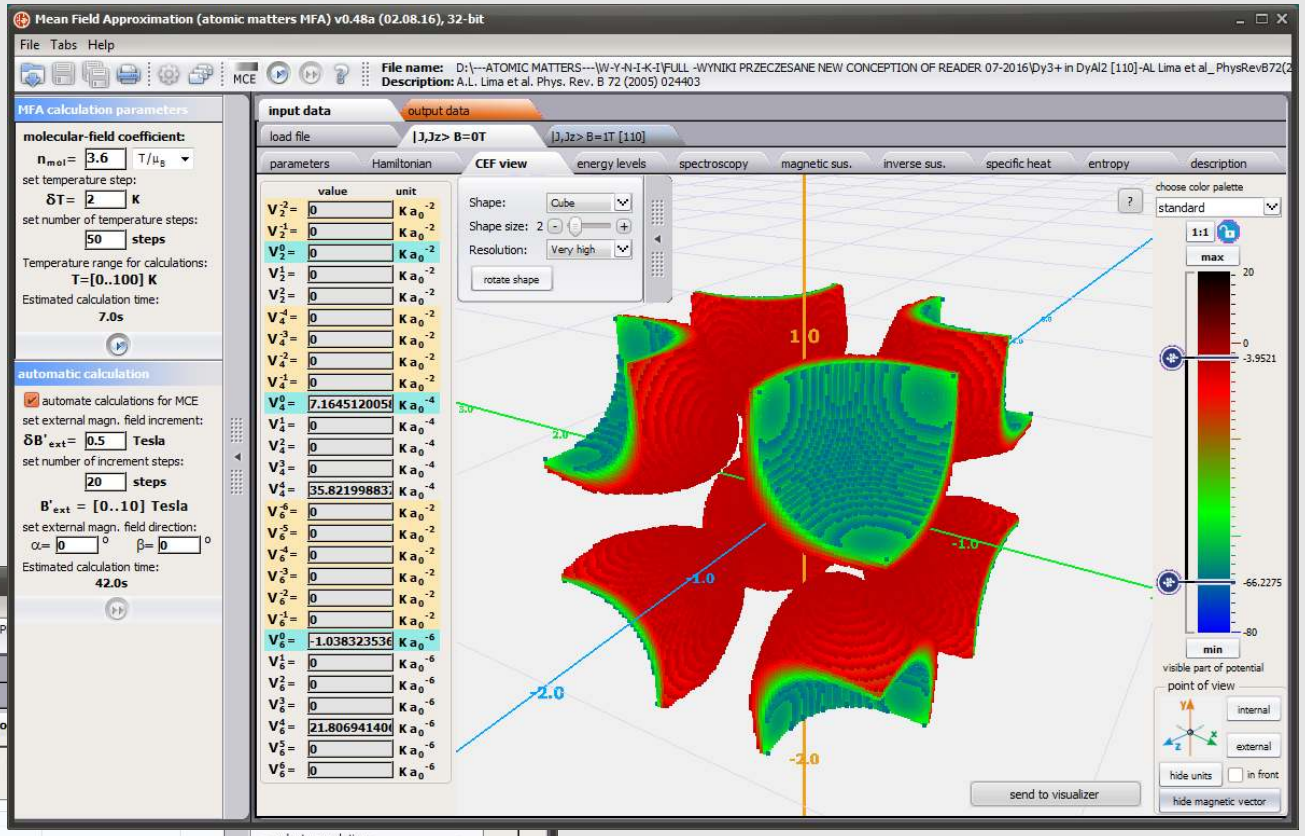


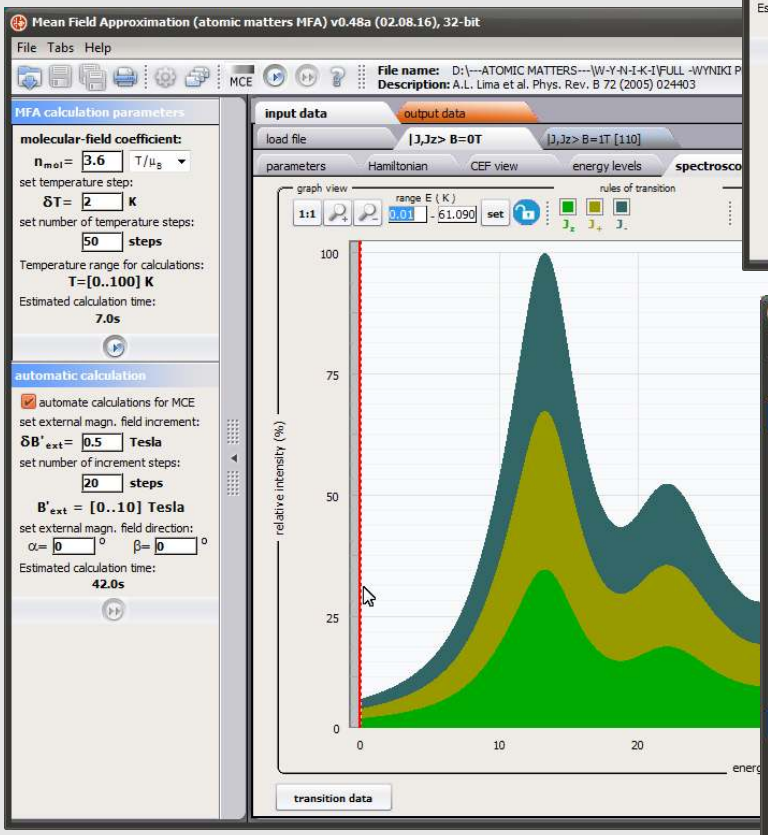
import parameters and settings from defined *.atma file

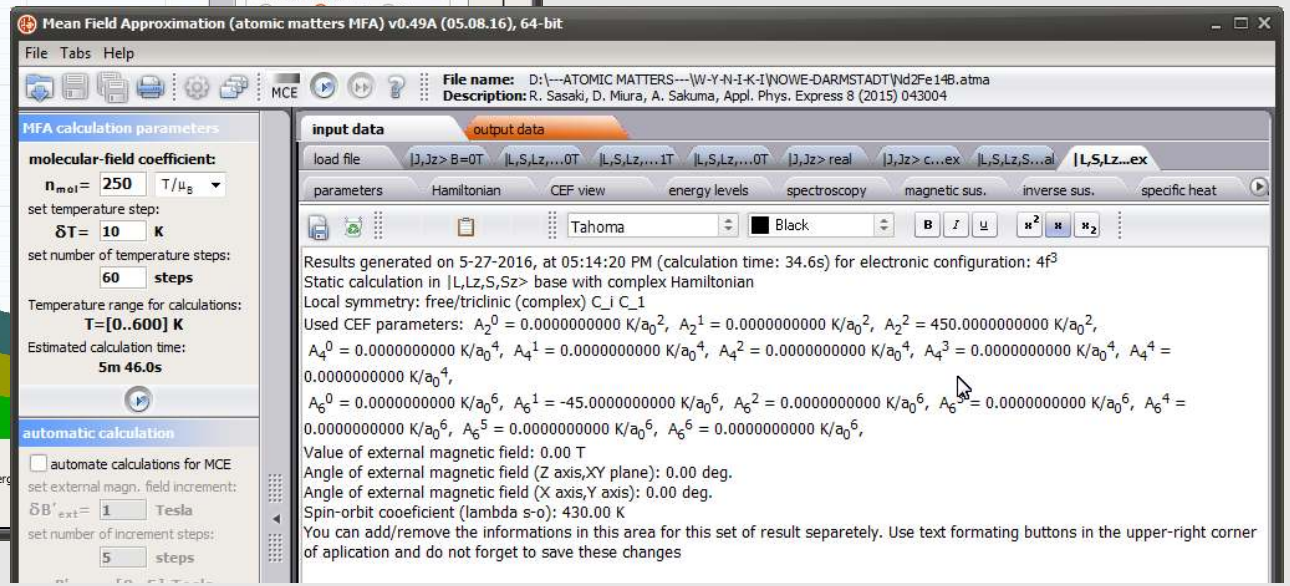
INPUT DATA - parameters calculation verification

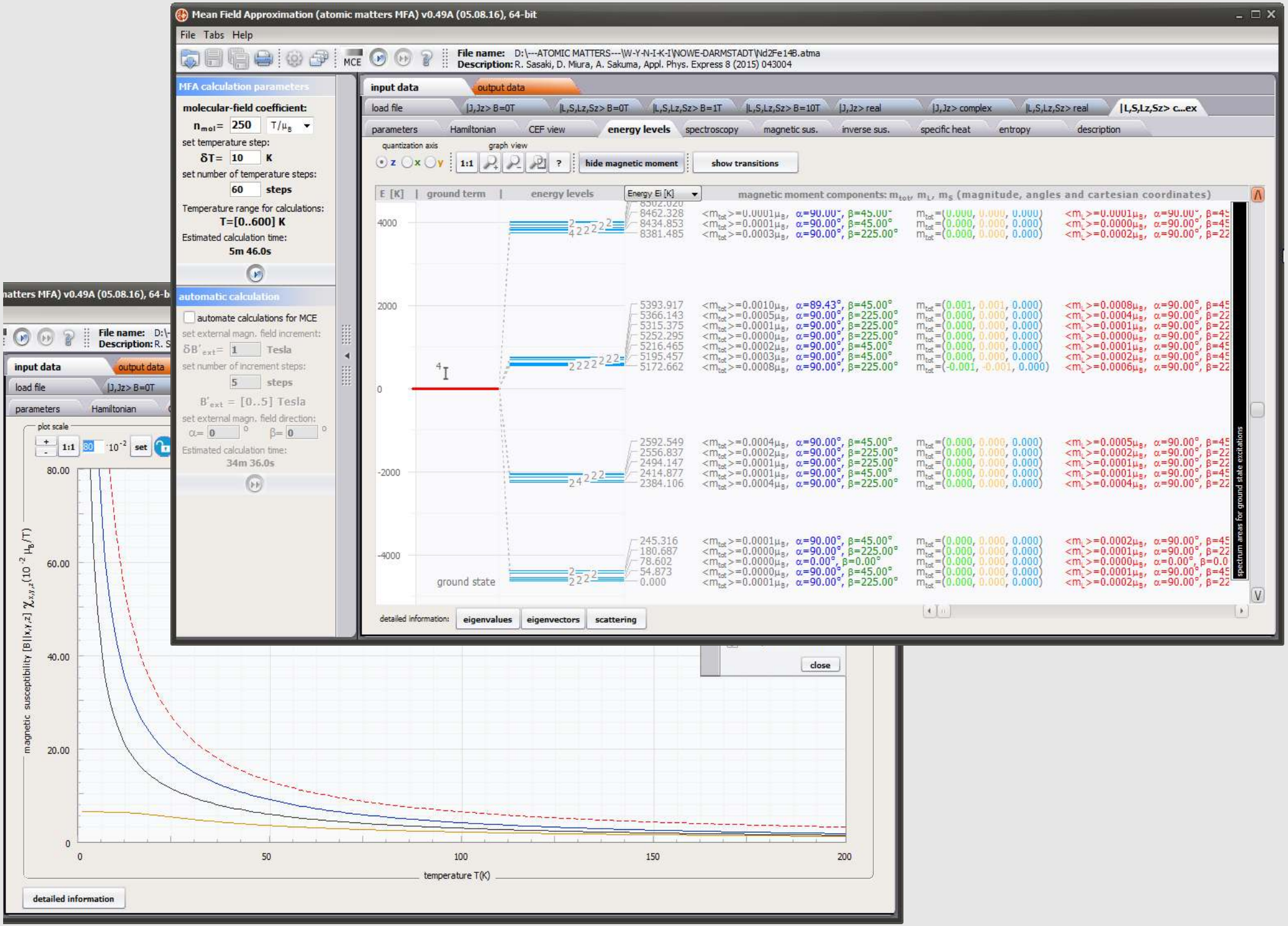
for Mean Field Approximation calculations

All result data from *.atma files is available in sub-tabs grouped in the 'input data' tab. All graph functionality is exactly the same as in corresponding tabs in Atomic Matters application. The set of results from an *.atma file that will be the source of parameters for MFA calculations can be chosen by setting the active input tab. Information about the number of calculation steps can be set on the left sliding panel. Estimated calculation time is shown.



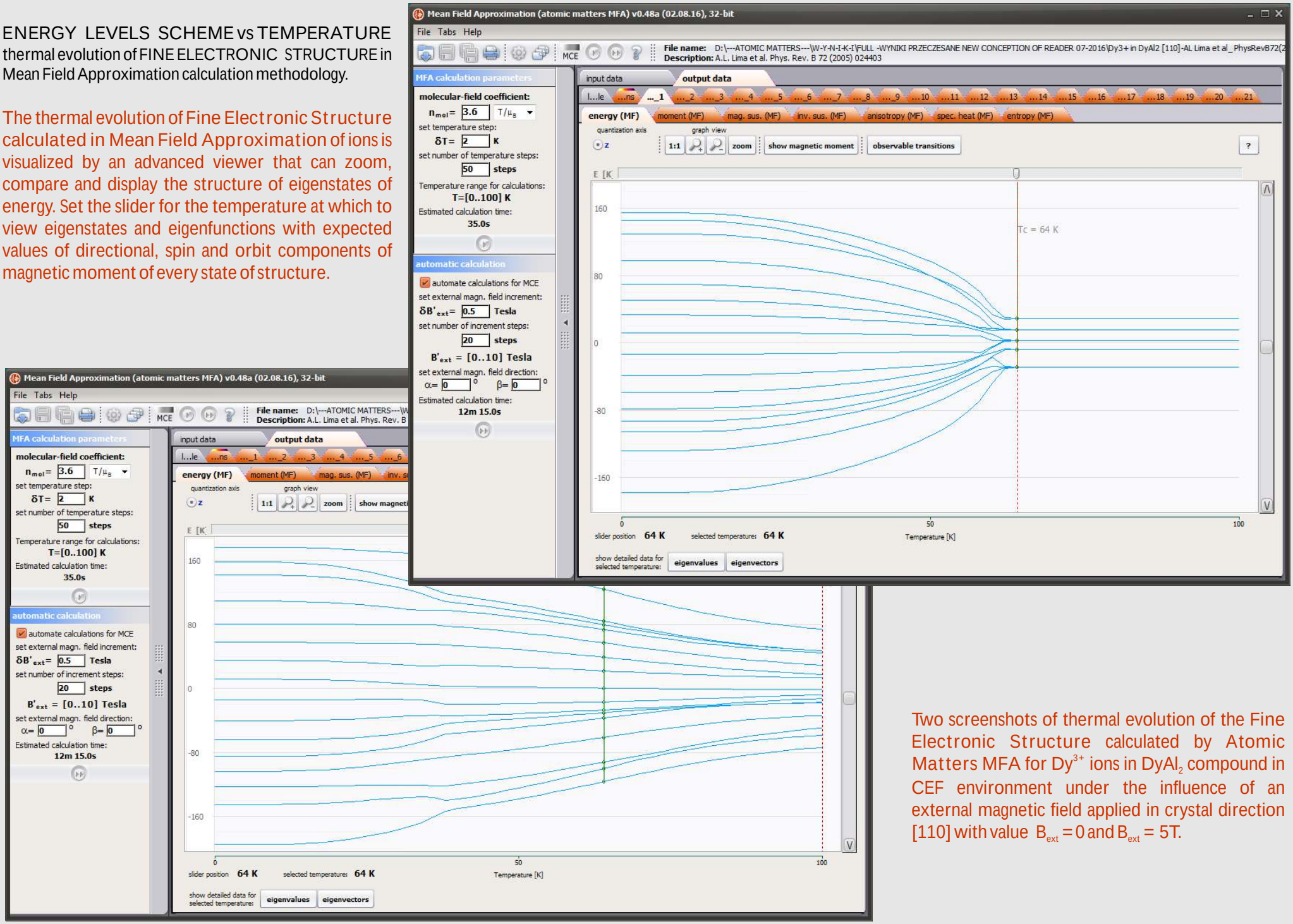





Mean Field Approximation (atomic matters MFA) v0.49A (05.08.16), 64-bit
File Tabs Help
File name: D:\---ATOMIC MATTERS---\W-Y-N-I-K-I\NOWE-DARMSTADT\Nd2Fe14B.atma
Description: R. Sasaki, D. Miura, A. Sakuma, Appl. Phys. Express 8 (2015) 043004
MFA calculation parameters
molecular-field coefficient:
n_mol= 250 T/μB
set temperature step:
δT= 10 K
set number of temperature steps:
60 steps
Temperature range for calculations:
T=[0..600] K
Estimated calculation time:
5m 46.0s
automatic calculation
automate calculations for MCE
set external magn. field increment:
δB'ext= 1 Tesla
set number of increment steps:
5 steps
B'ext = [0..5] Tesla
set external magn. field direction:
α= 0 ° β= 0 °
Estimated calculation time:
34m 36.0s
input data
output data
load file
|J,Jz> B=0T
|L,S,Lz,Sz> B=0T
|L,S,Lz,Sz> B=1T
|L,S,Lz,Sz> B=10T
|J,Jz> real
|J,Jz> complex
|L,S,Lz,Sz> real
|L,S,Lz,Sz> c...ex
parameters
Hamiltonian
CEF view
energy levels
spectroscopy
magnetic sus.
inverse sus.
specific heat
entropy
description
quantization axis
graph view
hide magnetic moment
show transitions
E [K]
ground term
energy levels
Energy Ei [K]
magnetic moment components: m_tot, m_L, m_S (magnitude, angles and cartesian coordinates)
ground state
spectrum areas for ground state excitations
detailed information:
eigenvalues
eigenvectors
scattering
plot scale
set
magnetic susceptibility [B||x,y,z] χx,y,z (10^-2 μB/T)
temperature T(K)
close
detailed information

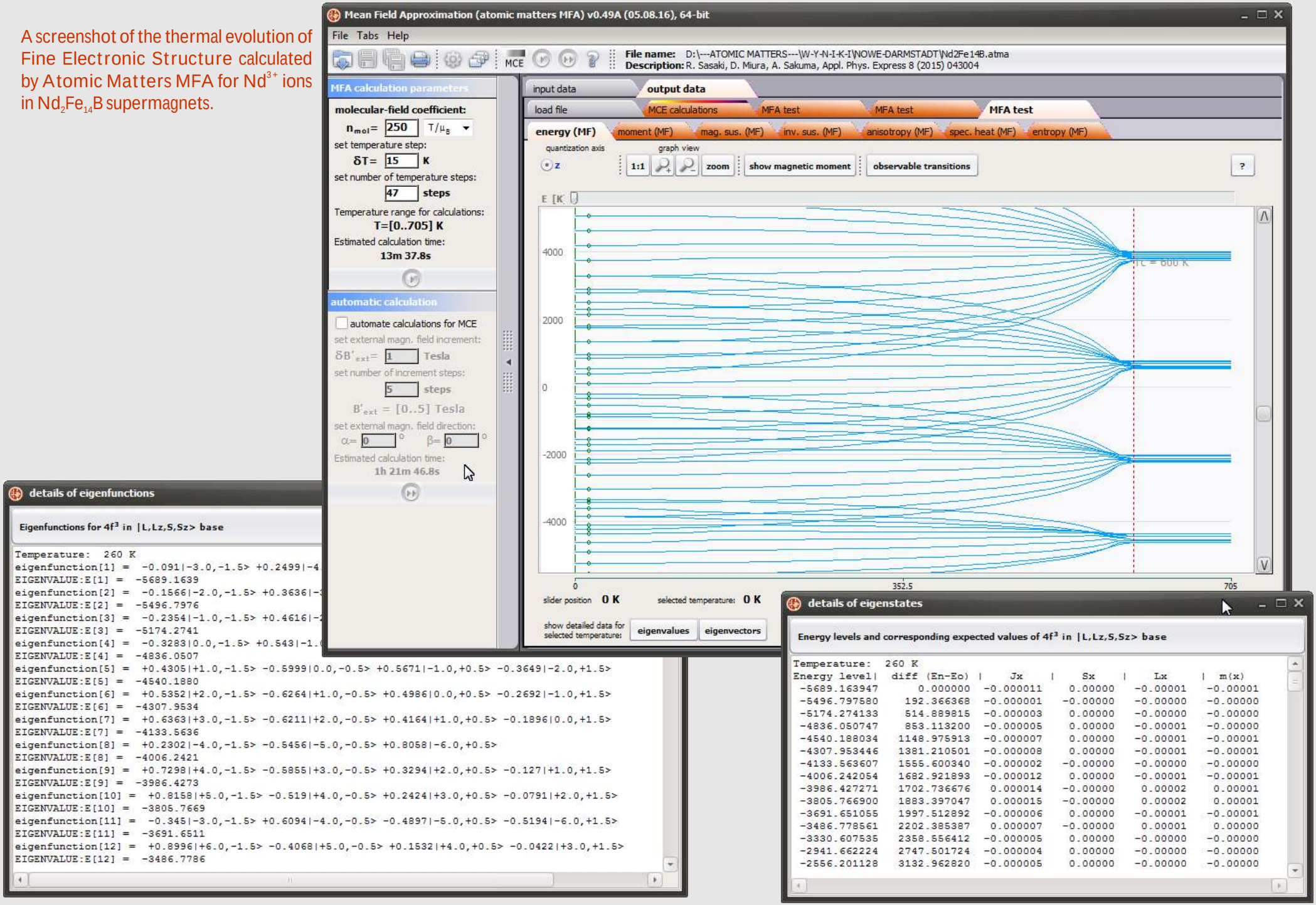
ENERGY LEVELS SCHEME vs TEMPERATURE
thermal evolution of FINE ELECTRONIC STRUCTURE in Mean Field Approximation calculation methodology.

The thermal evolution of Fine Electronic Structure calculated in Mean Field Approximation of ions is visualized by an advanced viewer that can zoom, compare and display the structure of eigenstates of energy. Set the slider for the temperature at which to view eigenstates and eigenfunctions with expected values of directional, spin and orbit components of magnetic moment of every state of structure.



Two screenshots of thermal evolution of the Fine Electronic Structure calculated by Atomic Matters MFA for Dy^{3+} ions in $DyAl_2$ compound in CEF environment under the influence of an external magnetic field applied in crystal direction [110] with value $B_{ext} = 0$ and $B_{ext} = 5T$.

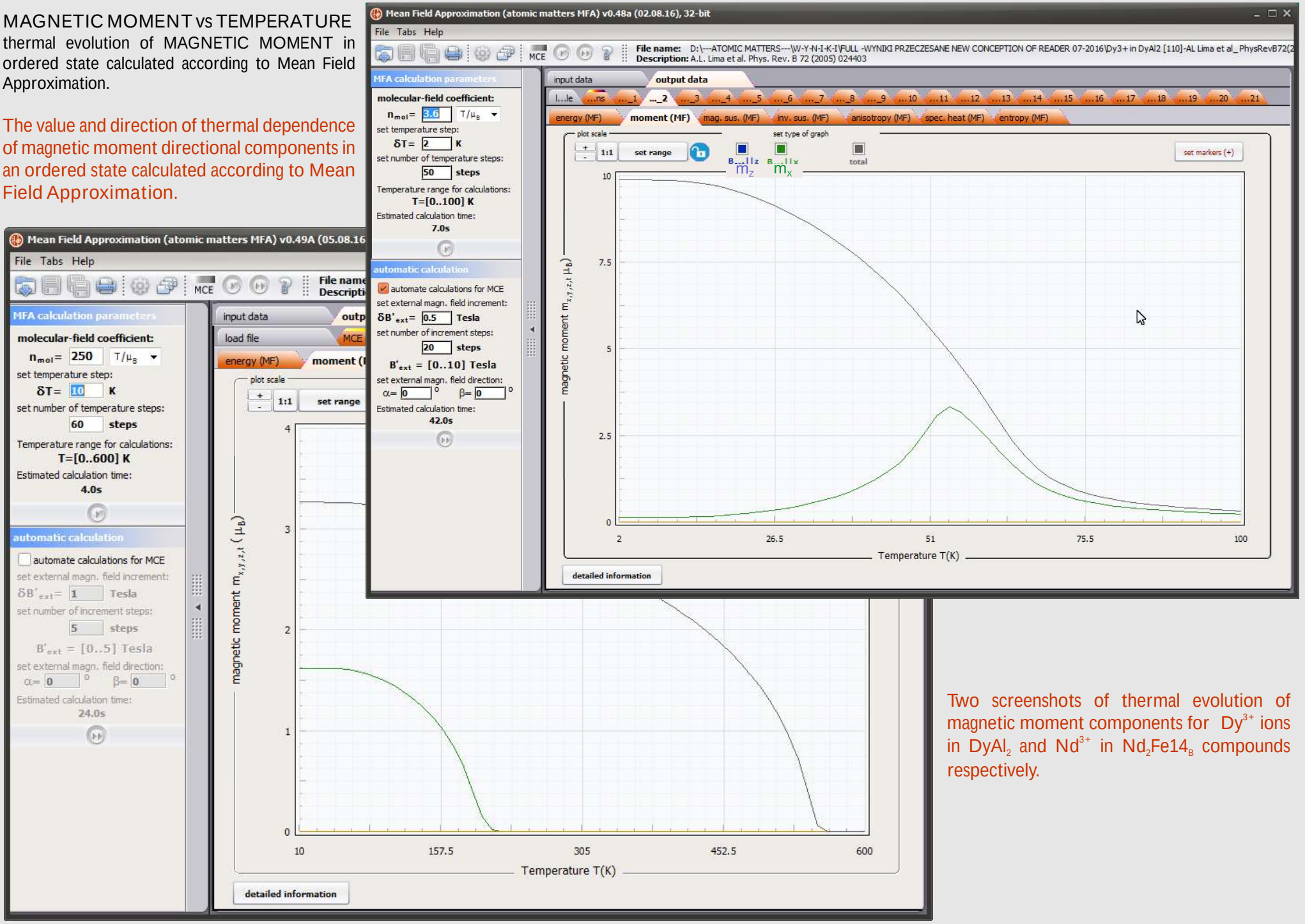
A screenshot of the thermal evolution of Fine Electronic Structure calculated by Atomic Matters MFA for Nd^{3+} ions in $Nd_2Fe_{14}B$ supermagnets.



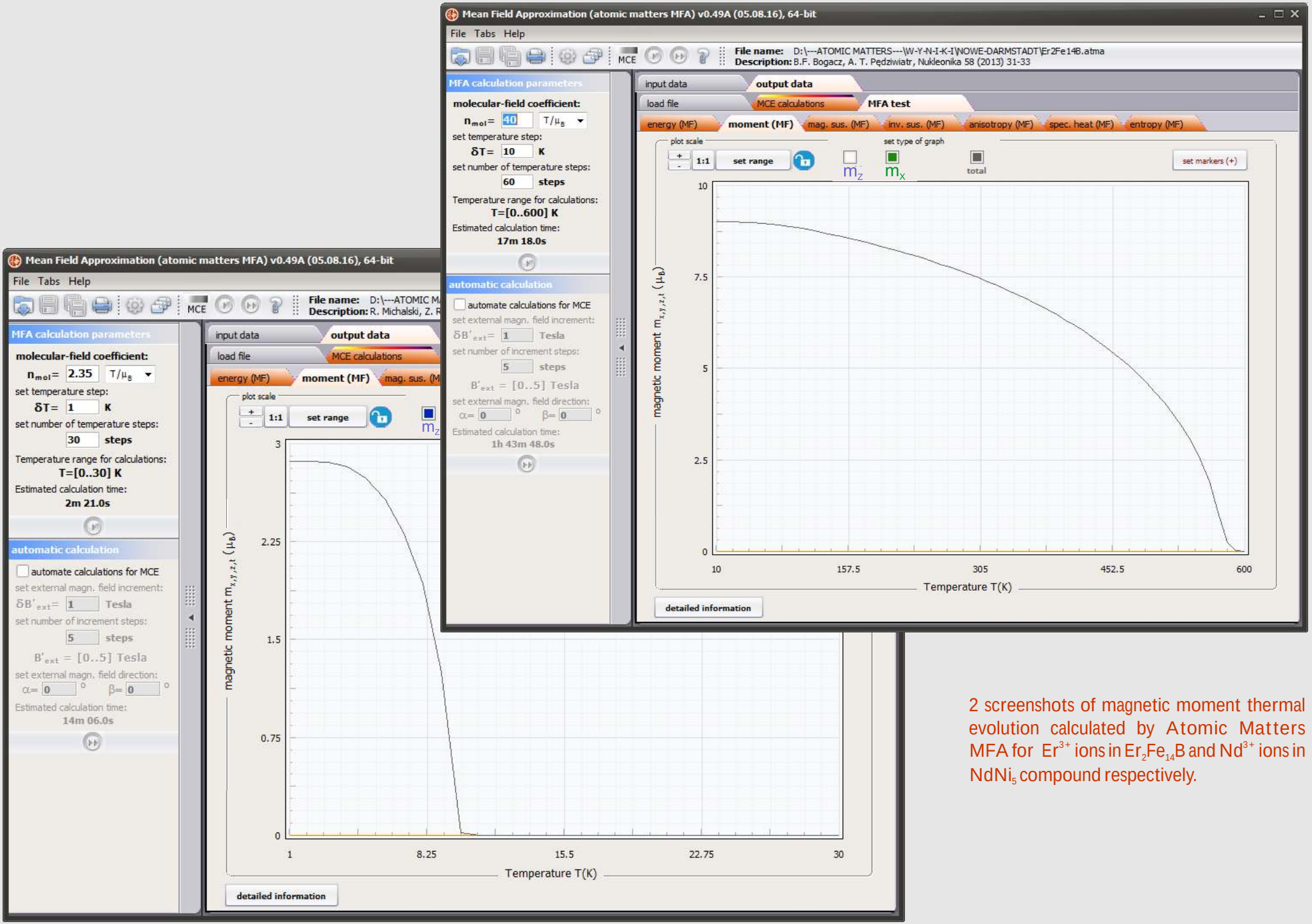
MAGNETIC MOMENT vs TEMPERATURE

thermal evolution of MAGNETIC MOMENT in ordered state calculated according to Mean Field Approximation.

The value and direction of thermal dependence of magnetic moment directional components in an ordered state calculated according to Mean Field Approximation.



Two screenshots of thermal evolution of magnetic moment components for Dy^{3+} ions in $DyAl_2$ and Nd^{3+} in Nd_2Fe14_B compounds respectively.



2 screenshots of magnetic moment thermal evolution calculated by Atomic Matters MFA for Er^{3+} ions in $Er_2Fe_{14}B$ and Nd^{3+} ions in $NdNi_5$ compound respectively.

MAGNETOCRYSTALLINE ANISOTROPY CONSTANTS $K_i(T)$ calculated according to Mean Field Approximation.

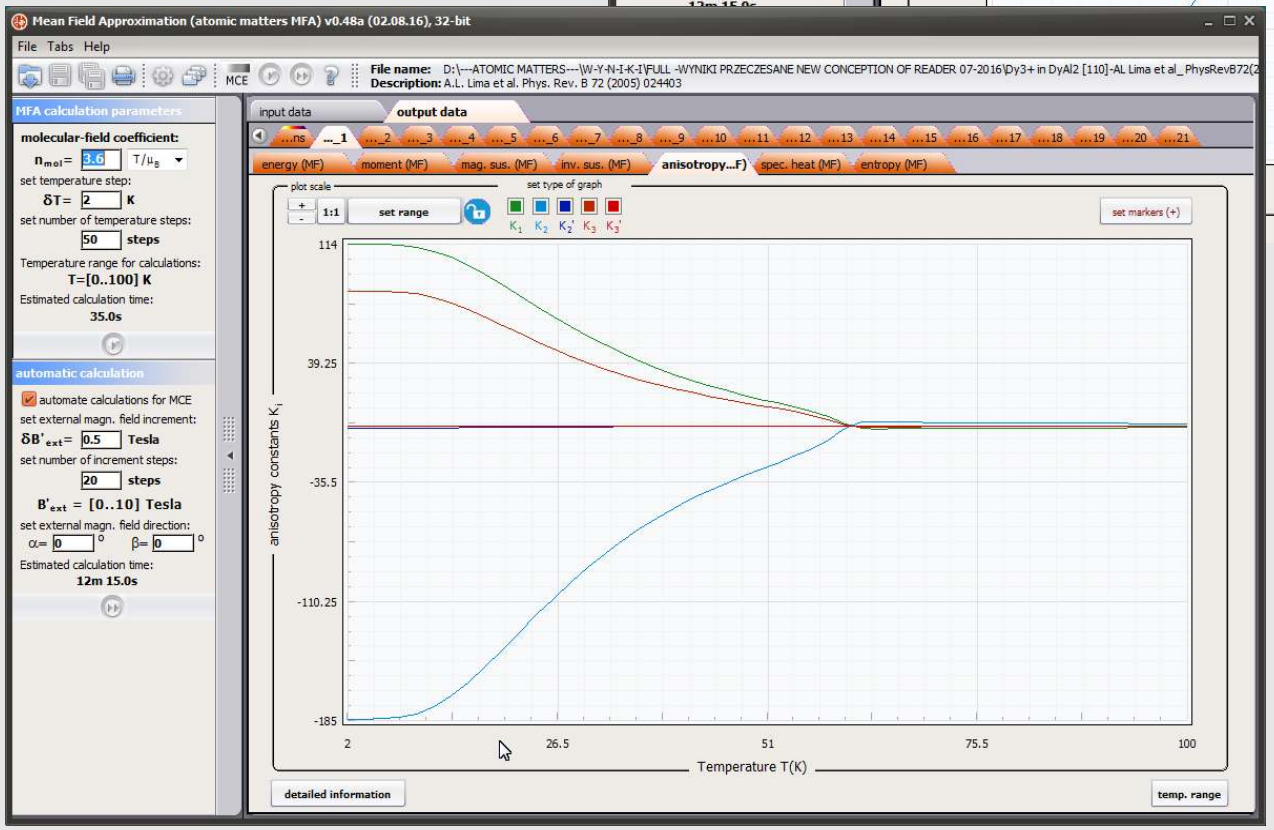
The value of magnetocrystalline constants K_i calculated for all temperatures from a defined region as expressions of Stevens operators $\langle O^n_m \rangle_T$ according to exact formulas:

$$K_1(T) = -\left(\frac{3}{2}B_2^0\langle\hat{O}_2^0\rangle + 5B_4^0\langle\hat{O}_4^0\rangle + \frac{21}{2}B_6^0\langle\hat{O}_6^0\rangle\right),$$

$$K_2(T) = \frac{7}{8}(5B_4^0\langle\hat{O}_4^0\rangle + 27B_6^0\langle\hat{O}_6^0\rangle),$$

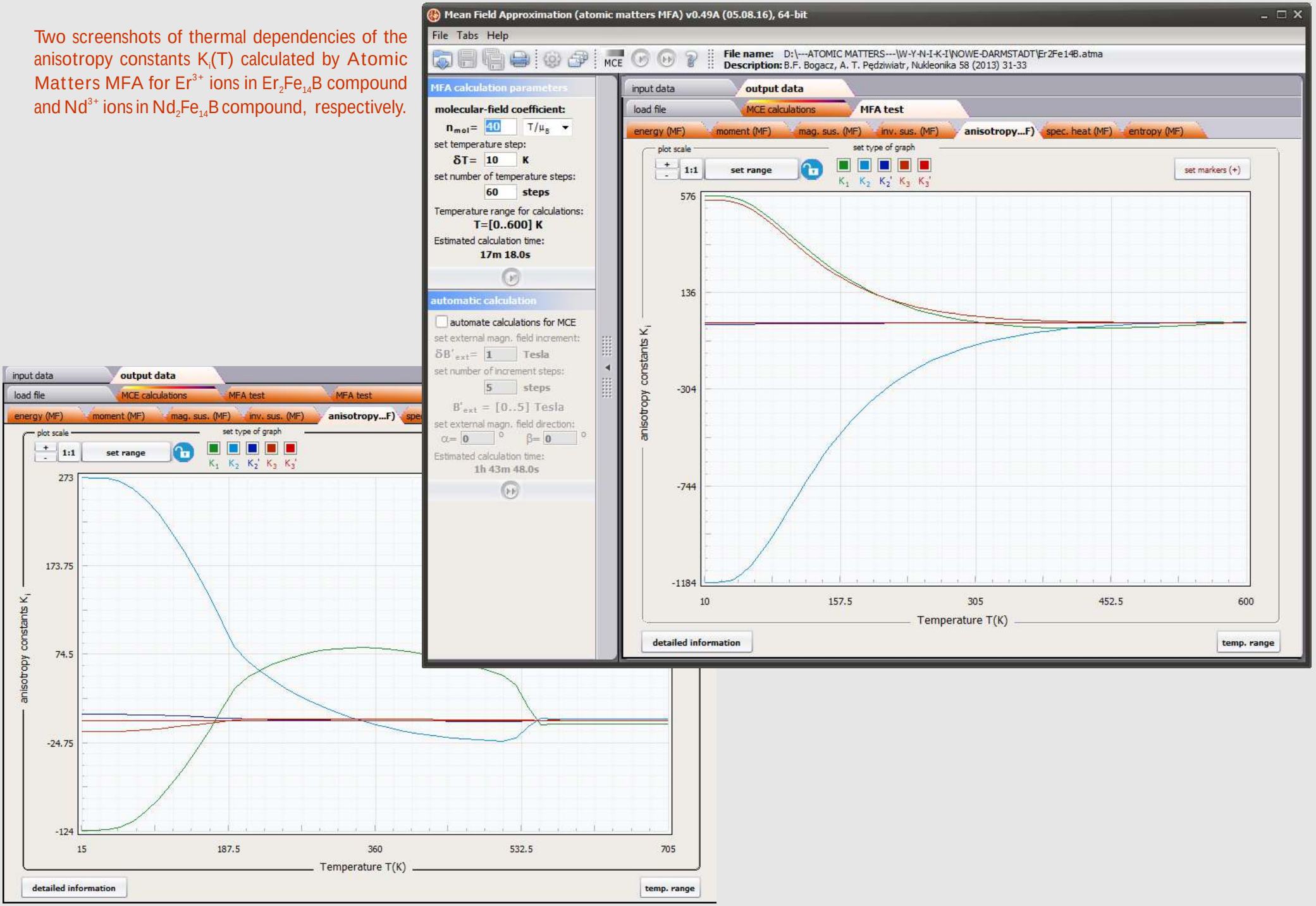
$$K_2^*(T) = \frac{1}{8}(B_4^0\langle\hat{O}_4^0\rangle + 5B_6^4\langle\hat{O}_6^4\rangle),$$

$$K_3(T) = -\frac{231}{16}B_6^0\langle\hat{O}_6^0\rangle,\ K_3^*(T) = -\frac{11}{16}B_6^4\langle\hat{O}_6^4\rangle.$$



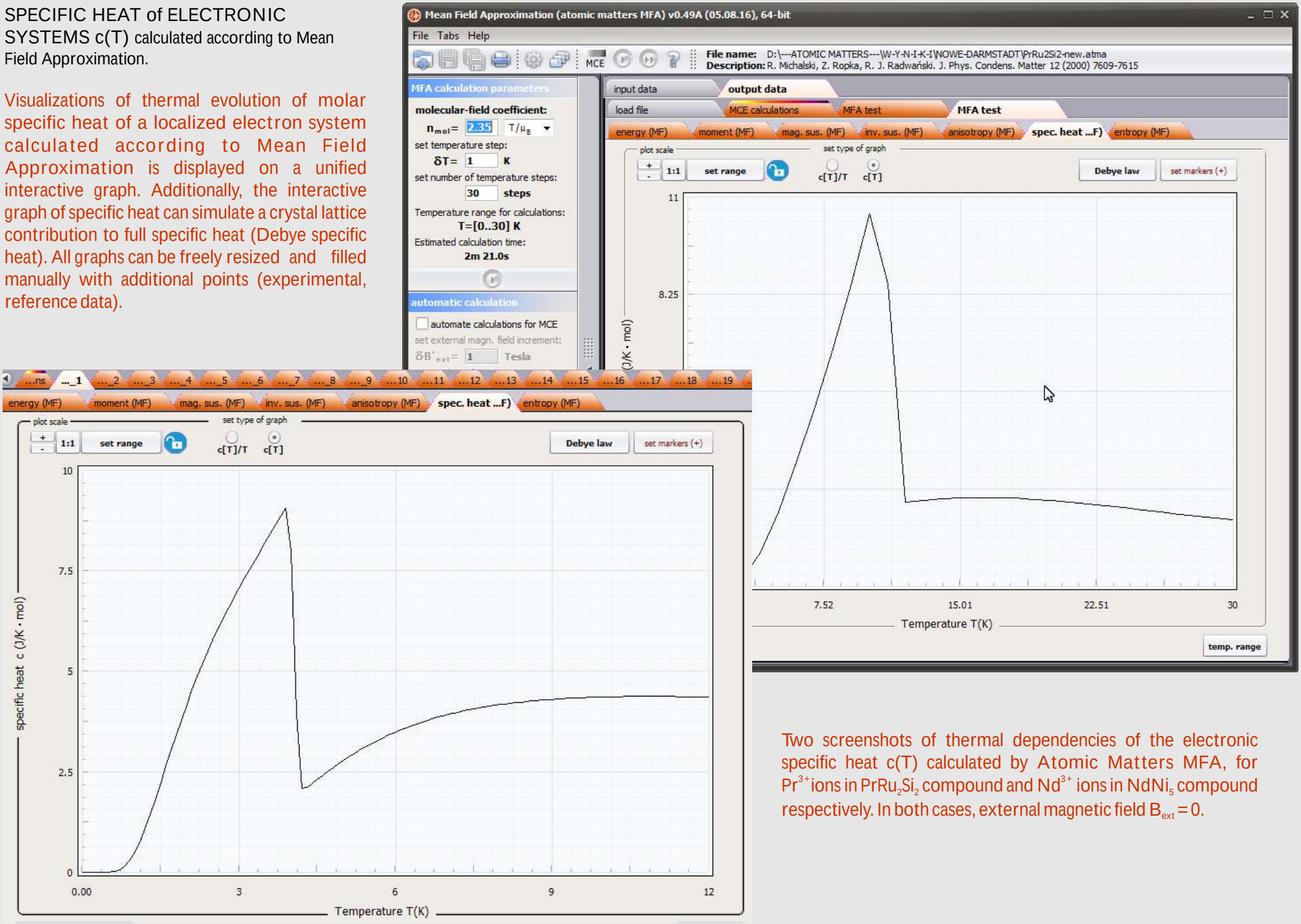
Two screenshots of thermal dependencies of the anisotropy constants $K_i(T)$ calculated by Atomic Matters MFA for Dy^{3+} ions in $DyAl_2$ compound in a CEF environment under the influence of an external magnetic field applied in crystal direction [100] with value $B_{ext} = 0$ and $B_{ext} = 5T$ respectively.

Two screenshots of thermal dependencies of the anisotropy constants $K_i(T)$ calculated by Atomic Matters MFA for Er^{3+} ions in $Er_2Fe_{14}B$ compound and Nd^{3+} ions in $Nd_2Fe_{14}B$ compound, respectively.



SPECIFIC HEAT of ELECTRONIC SYSTEMS c(T) calculated according to Mean Field Approximation.

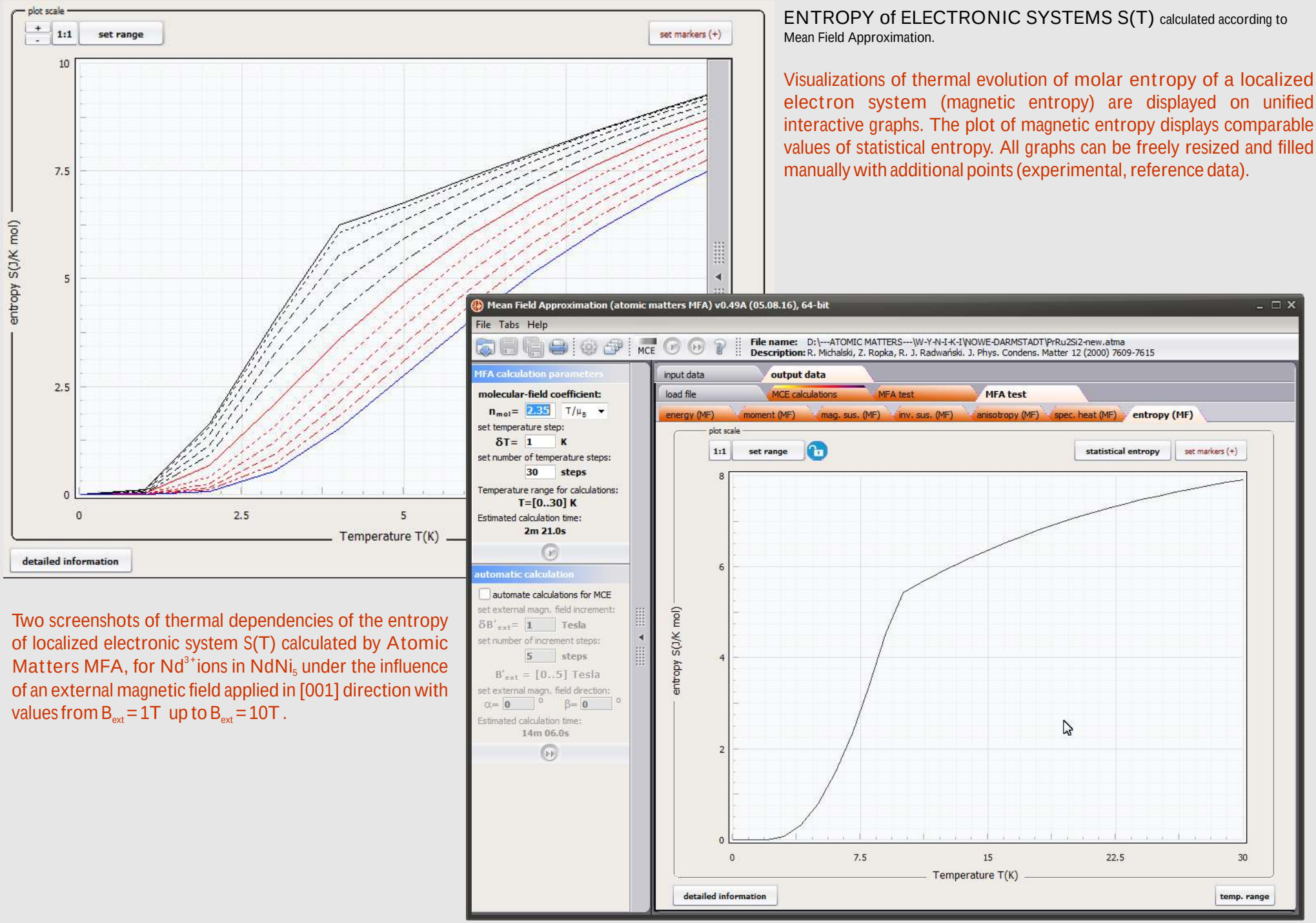
Visualizations of thermal evolution of molar specific heat of a localized electron system calculated according to Mean Field Approximation is displayed on a unified interactive graph. Additionally, the interactive graph of specific heat can simulate a crystal lattice contribution to full specific heat (Debye specific heat). All graphs can be freely resized and filled manually with additional points (experimental, reference data).



Two screenshots of thermal dependencies of the electronic specific heat c(T) calculated by Atomic Matters MFA, for Pr^{3+} ions in $PrRu_2Si_2$ compound and Nd^{3+} ions in $NdNi_5$ compound respectively. In both cases, external magnetic field $B_{ext} = 0$.

ENTROPY of ELECTRONIC SYSTEMS S(T) calculated according to Mean Field Approximation.

Visualizations of thermal evolution of molar entropy of a localized electron system (magnetic entropy) are displayed on unified interactive graphs. The plot of magnetic entropy displays comparable values of statistical entropy. All graphs can be freely resized and filled manually with additional points (experimental, reference data).

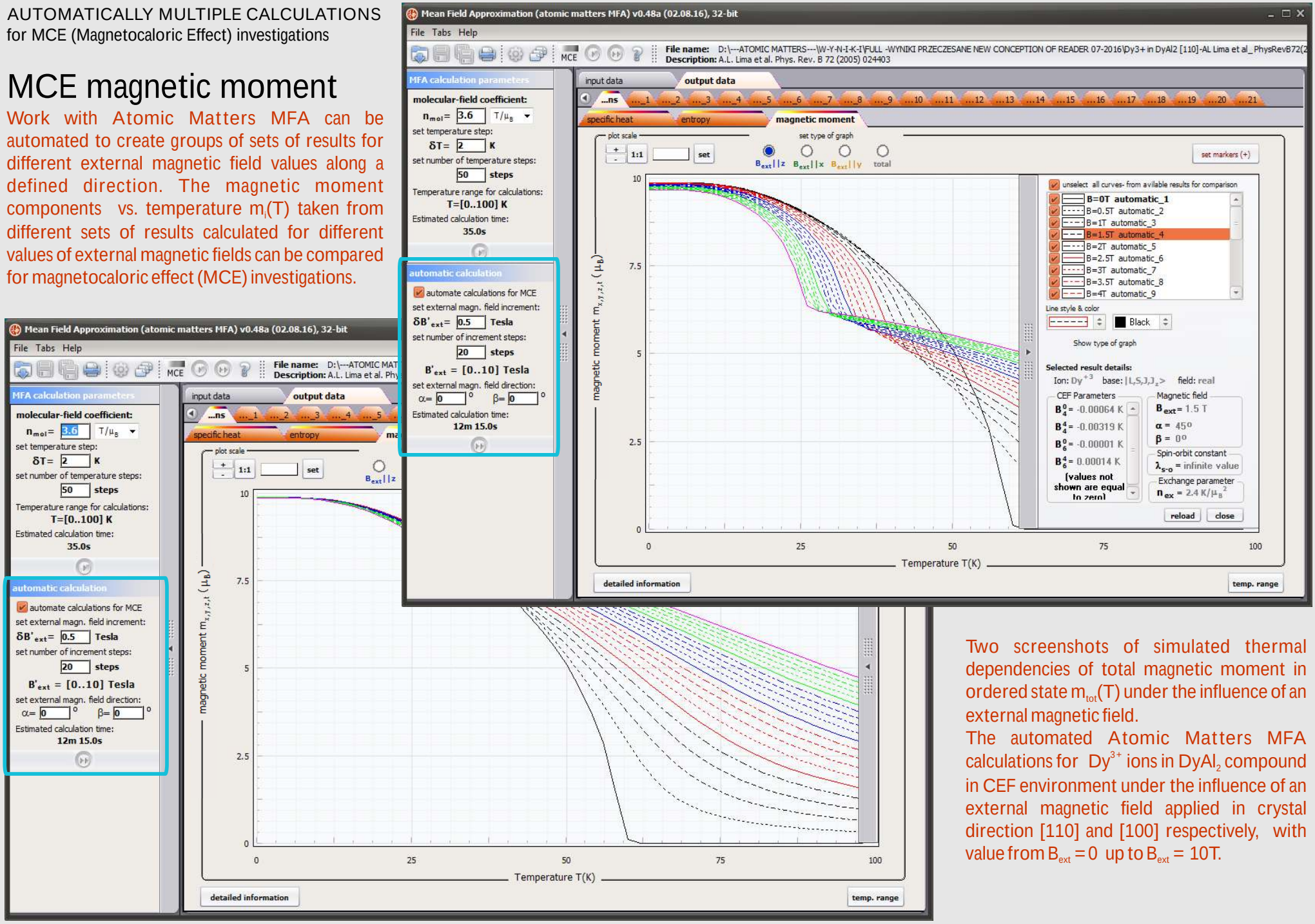


Two screenshots of thermal dependencies of the entropy of localized electronic system S(T) calculated by Atomic Matters MFA, for Nd^{3+} ions in $NdNi_5$ under the influence of an external magnetic field applied in [001] direction with values from $B_{ext} = 1T$ up to $B_{ext} = 10T$.

AUTOMATICALLY MULTIPLE CALCULATIONS
for MCE (Magnetocaloric Effect) investigations

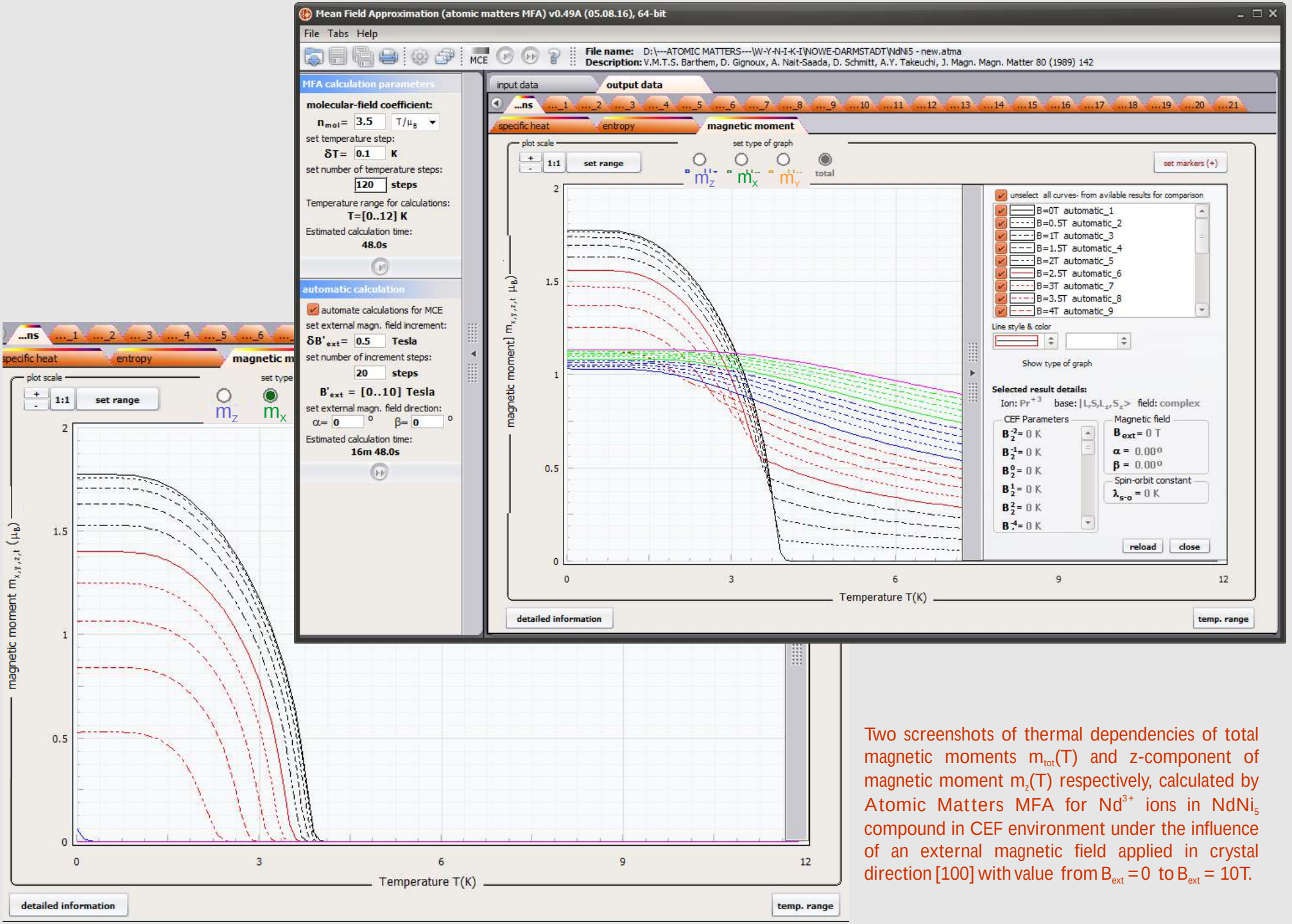
MCE magnetic moment

Work with Atomic Matters MFA can be automated to create groups of sets of results for different external magnetic field values along a defined direction. The magnetic moment components vs. temperature $m_i(T)$ taken from different sets of results calculated for different values of external magnetic fields can be compared for magnetocaloric effect (MCE) investigations.



Two screenshots of simulated thermal dependencies of total magnetic moment in ordered state $m_{tot}(T)$ under the influence of an external magnetic field.

The automated Atomic Matters MFA calculations for Dy^{3+} ions in $DyAl_2$ compound in CEF environment under the influence of an external magnetic field applied in crystal direction [110] and [100] respectively, with value from $B_{ext} = 0$ up to $B_{ext} = 10T$.

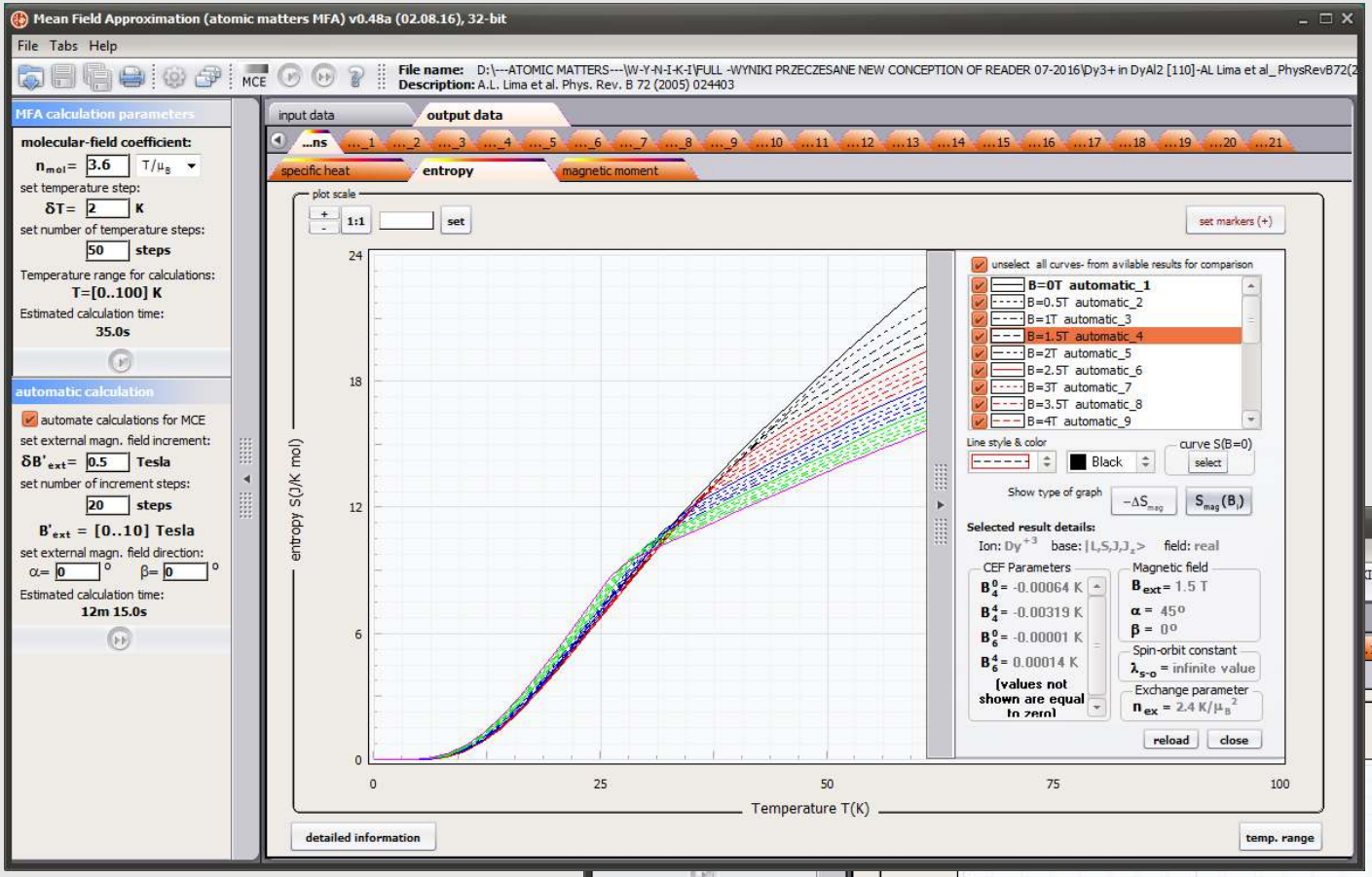


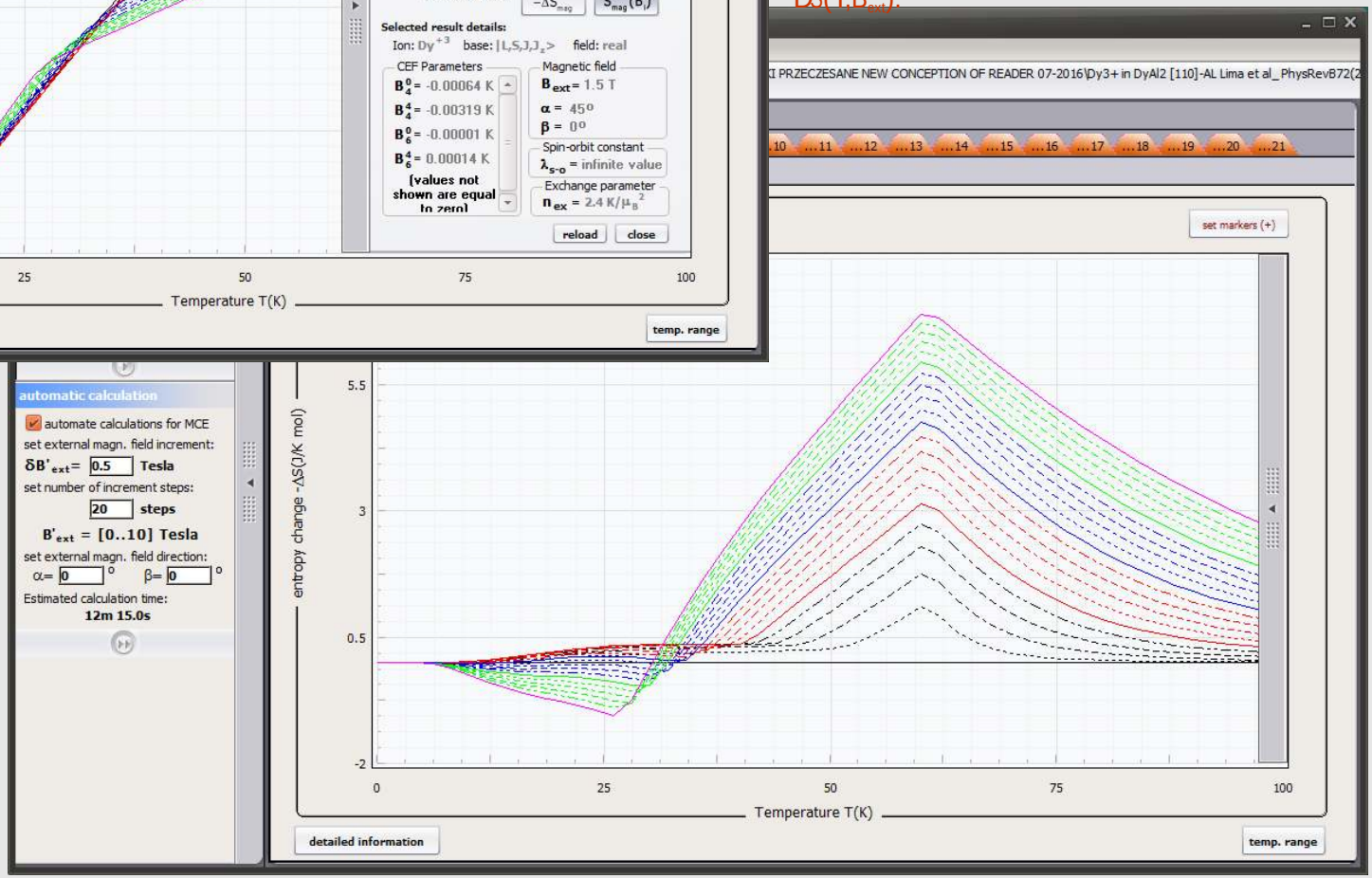
Two screenshots of thermal dependencies of total magnetic moments $m_{tot}(T)$ and z-component of magnetic moment $m_z(T)$ respectively, calculated by Atomic Matters MFA for Nd^{3+} ions in $NdNi_5$ compound in CEF environment under the influence of an external magnetic field applied in crystal direction [100] with value from $B_{ext} = 0$ to $B_{ext} = 10T$.

MAGNETOCALORIC EFFECT
and AUTOMATION of multiple MFA CALCULATIONS

MCE entropy

Entropy curves $S_{mag}(T,B_{ext})$ taken from different result sets calculated for different values of an external magnetic field can be compared and transformed for magnetocaloric effect (MCE) investigations. The entropy curves can be taken from result sets calculated separately or by using MCE automation. Select the curve $S(T,0)$ for $B_{ext}=0$ and subtract it from other curves $S(T,B_{ext})$ to demonstrate magnetocaloric effect parameter $DS(T,B_{ext})$.



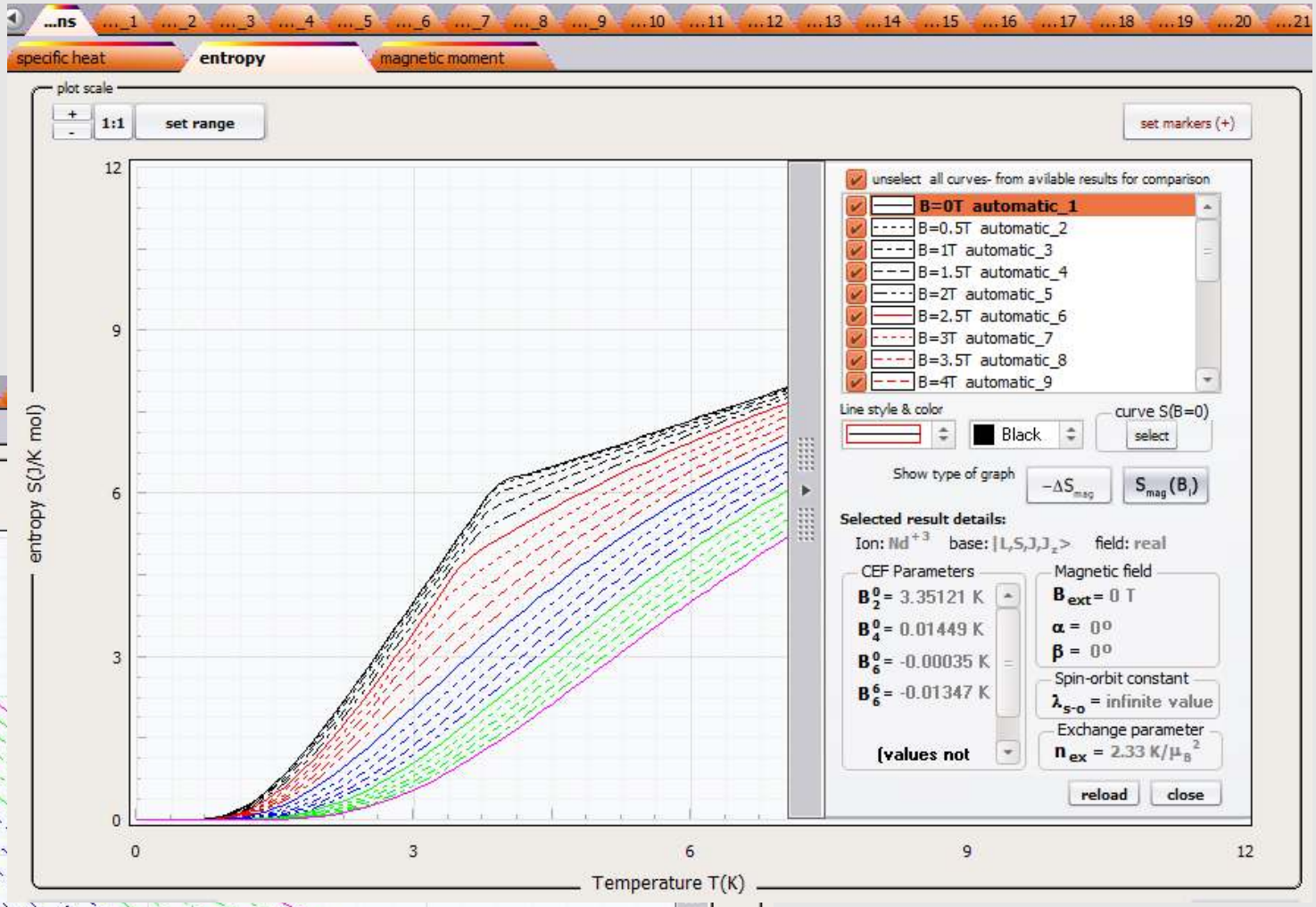


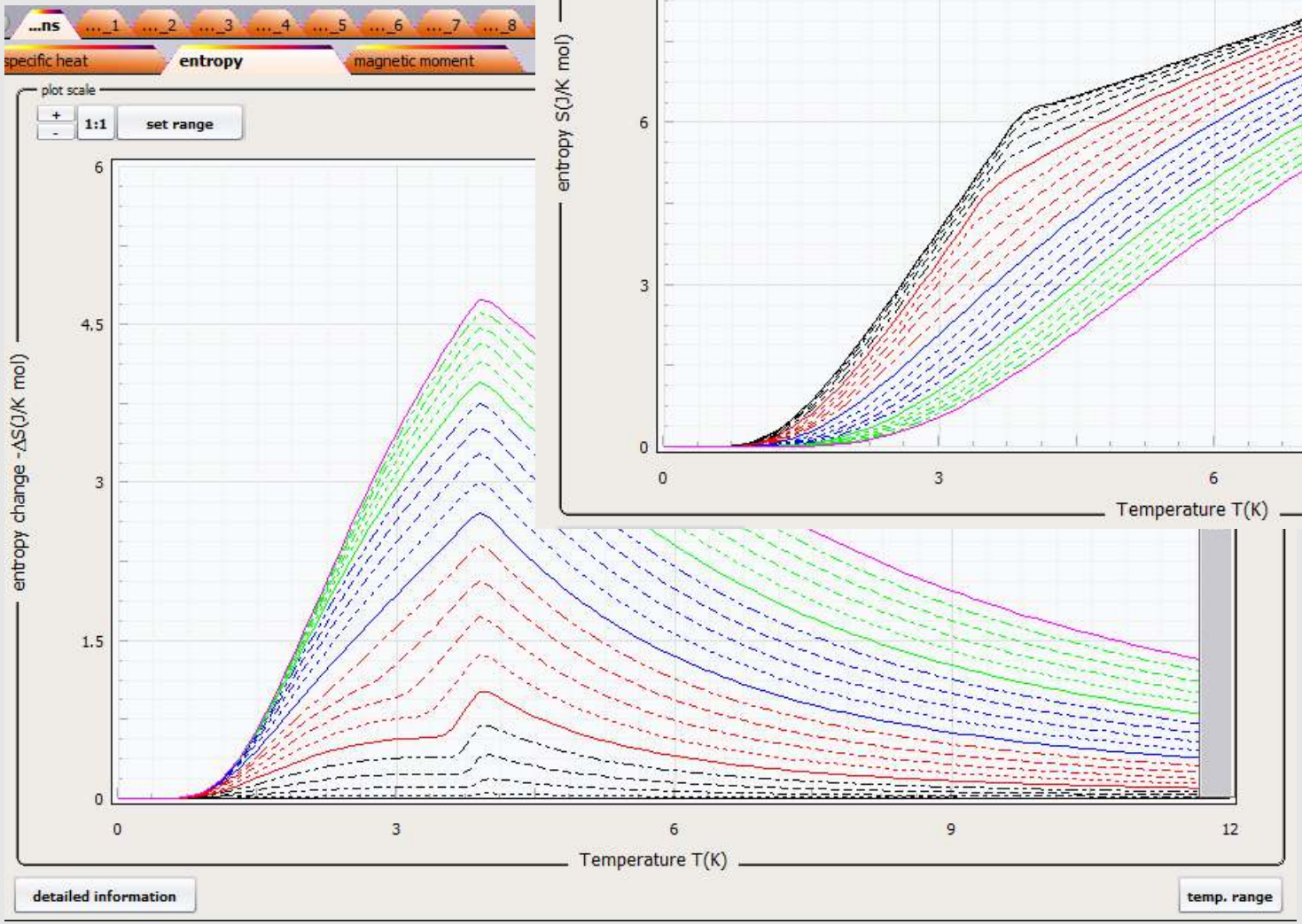
Two MCE entropy screenshots: thermal dependencies of entropy $S(T,B_{ext})$ and entropy change parameter $-DS(T,B_{ext})$, respectively.

The automated Atomic Matters MFA calculations for Dy^{3+} ions in $DyAl_2$ compound in a CEF environment under the influence of an external magnetic field applied in crystal direction [110], with value from $B_{ext}=0$ up to $B_{ext}=10T$.

Two MCE entropy screenshots for the automated Atomic Matters MFA calculations for Nd^{3+} ions in $NdNi_5$ compound in a CEF environment under the influence of an external magnetic field applied in crystal direction [001], with value from $B_{ext} = 0$ up to $B_{ext} = 10T$.

The screenshots show the thermal dependencies of entropy $S(T,B_{ext})$ and MCE entropy change parameter $-DS(T,B_{ext})$, respectively.

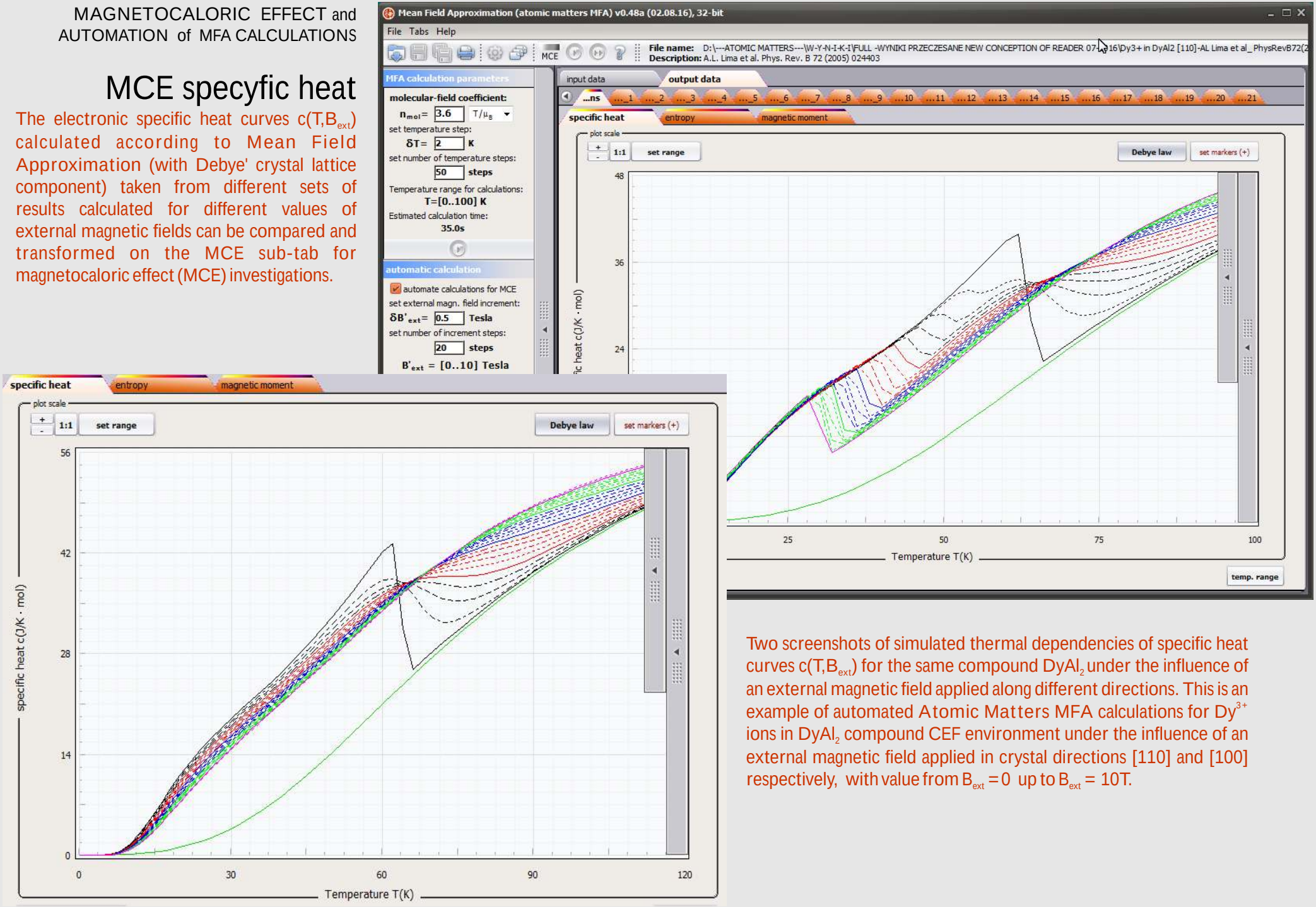




MAGNETOCALORIC EFFECT and
AUTOMATION of MFA CALCULATIONS

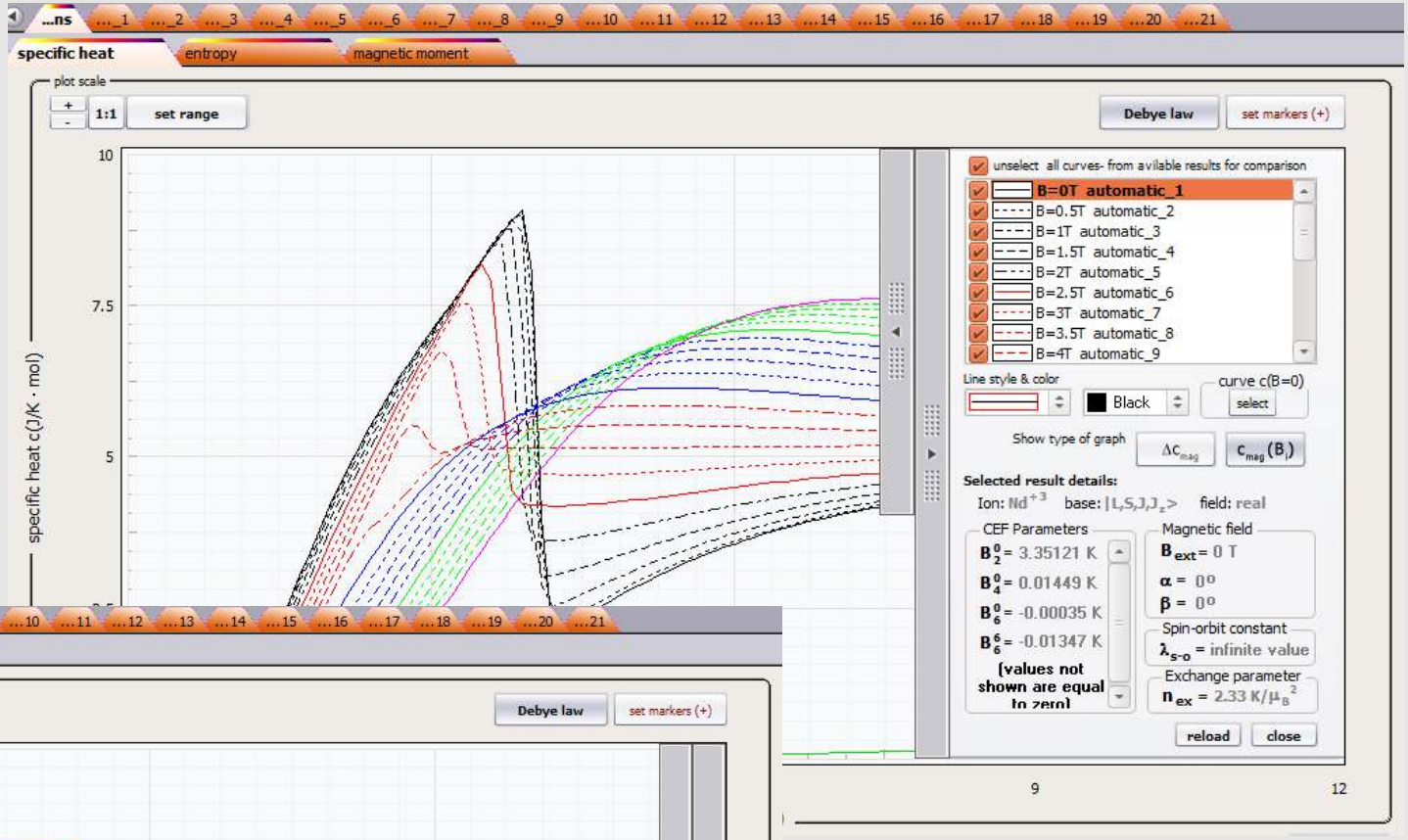
MCE specyfic heat

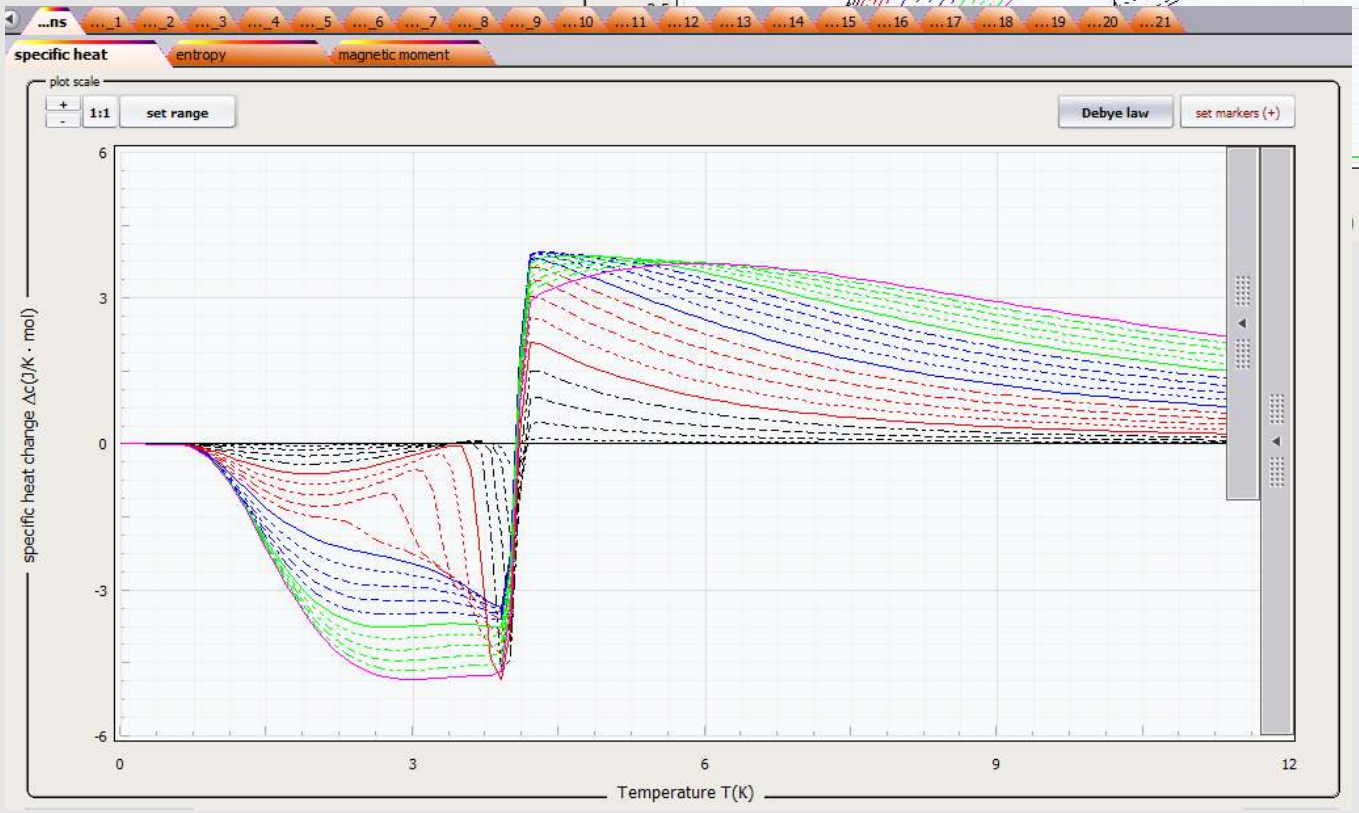
The electronic specific heat curves $c(T,B_{ext})$ calculated according to Mean Field Approximation (with Debye' crystal lattice component) taken from different sets of results calculated for different values of external magnetic fields can be compared and transformed on the MCE sub-tab for magnetocaloric effect (MCE) investigations.



Two screenshots of simulated thermal dependencies of specific heat curves $c(T,B_{ext})$ for the same compound $DyAl_2$ under the influence of an external magnetic field applied along different directions. This is an example of automated Atomic Matters MFA calculations for Dy^{3+} ions in $DyAl_2$ compound CEF environment under the influence of an external magnetic field applied in crystal directions [110] and [100] respectively, with value from $B_{ext} = 0$ up to $B_{ext} = 10T$.

Calculated thermal dependencies of specific heat for Nd^{3+} ions in $NdNi_5$. The screenshots show specific heat curves $c(T,B_{ext})$ and specific heat change $Dc(T,B_{ext})$ transformed from $c(T,B_{ext})$ by subtracting $c(T,B_{ext}=0)$.
An external magnetic field was applied along [001], with value from $B_{ext}=0$ up to $B_{ext}=10T$.





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