atomic matters atomic properties and magnetism of solids atomic matters MFA Mean Field Approximation atomic computation system



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 userdefined 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

> > Rafa Michalski Atomic Matters project Leader









OPEN SELECTED

atma EII E

SET MOLECULAR

n_{mr}

YES

to:

T_i<DT

?

FIELD PARAMETER

Calculate population of states

for T_i=T_{i-1}+OT and calculate

Fill Hamiltonian matrix using:

CEF operator components (B^m, O^m).

if complex

CALCULATE EXPECTED VALUES OF

3 DIRECTIONAL COMPONENTS OF

field selected

Spin-orbit coupling interactions components (I s-oLS),

 $\mathbf{m}(T_i)$ for $\mathbf{B}_{moi}(T_{i+1})$

of various external magnetic fields Ber RESULT DATA STORE in INTERACTIVE COMPARISON *.mfa FILE EXPORT DATA VISUALISATIONS TOOL (MCE)



2 PCM CALCULATOR POINT CHARGE MODEL APPROXIMATION

Point Charge Model approximation is a useful

CRYSTA

FIELD (CEF)

STEVÈNS

PARAMETERS B

ARE KNOWN?

AVAILABLE

PRIMITIVE POINT-CHARGE SYMMETRIES

YES

POINT

CHARGE

MODEL

(PCM) ESTIMATI









parameters familities GF Hear encopy level pacebox reverse as specific levels decopies MARCE Letters Ma	periodic table potential visualizer [], Jz > real Hamiltonix [], Jz > complex Hamix [L,S,Lz,Sz > real Haix [L,S,Lz,Sz > compleix Result04											HAMILTONIAN	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	paramet	ers Ham	iltonian CE	F view	energy levels	spectroscopy	magnetic s	us. inverse	sus. spec	ific heat e	ntropy	descriptio	MATRIX ELEMENTS
L-93 0 <th></th> <th>Lz=5Sz=2.5</th> <th>Lz=5Sz=1.5</th> <th>Lz=5Sz=0.5</th> <th>Lz=5Sz=-0.5</th> <th>Lz=5Sz=-1.5</th> <th>Lz=5Sz=-2.5</th> <th>Lz=4Sz=2.5</th> <th>Lz=4Sz=1.5</th> <th>Lz=45z=0.5</th> <th>Lz=4Sz=-0.5</th> <th>Lz=4</th> <th>- Used parameters:</th>		Lz=5Sz=2.5	Lz=5Sz=1.5	Lz=5Sz=0.5	Lz=5Sz=-0.5	Lz=5Sz=-1.5	Lz=5Sz=-2.5	Lz=4Sz=2.5	Lz=4Sz=1.5	Lz=45z=0.5	Lz=4Sz=-0.5	Lz=4	- Used parameters:
	Lz=5 Sz=2.5	-6875	0	0	0	0	0	0	0	0	0	=	Flow anti: Di mara sium
9.7-20 53.5788 6.2211-4.768 0 </td <td>-69.93798</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td> <td>0.1647+4.92</td> <td>0</td> <td>0</td> <td>0</td> <td></td> <td>Z = 66</td>		-69.93798	0	0	0	0	0	0.1647+4.92	0	0	0		Z = 66
		35.37588	6.3211-4.763	0	0	0	0	4.4645-3.364	0	0	0		Oxidation: +3
	10 100	0	-4125	0	0	0	0	-1944.5436	0	0	0		Dimension: 66
year year 23.286 year 0 0 year 0 0 year 0 0 year 0 <td>Lz=5</td> <td>0</td> <td>-69.93798</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td> <td>0.1647+4.92i</td> <td>0</td> <td>0</td> <td></td> <td>Base: L,S,L_z,S_z></td>	Lz=5	0	-69.93798	0	0	0	0	0	0.1647+4.92i	0	0		Base: L,S,L _z ,S _z >
	52-1.5	XXXX	28.2966	7.9956-6.025	0	0	0	0	4.4645-3.364	0	0		Field: Complex
		0	0	-1375	0	0	0	0	-2459.6748	0	0		
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Lz=5	0	0	-69.93798	0	0	0	0	0	0.1647+4.92i	0		$\lambda_{so} = -550$
		0	XXXX	21.21731	8.4807-6.391	0	0	0	0	4.4645-3.364	0		B _x = 2.823603
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		0	0	0	<u>1375</u>	0	0	0	0	-2608.8791	0		$B_{\gamma} = 2.127737$
$ \ \ \ \ \ \ \ \ \ \ \ \ \$	Lz=5 Sz=-0.5	0	(0)	0	-69.93798	0	0	0	0	0	0.1647+4.92i		$B_z = 3.535534$
		0	0	XXXX	14.13803	7.9956-6.025	0	0		0	4.4645-3.364		
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		0	0	0	0	4125	0	0	0	0	-2459.6748		IS 0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Lz=5	0	0	0	0	-69.93798	0	0	0	0	0	0.164	V CEE 0 16473
		0	0	0	XXXX	7.05874	6.3211-4.763	0	0	0	0	4.464	+4.91965i
		0	0	0	0	0	<u>6875</u>	0	0	0	0	-194	Mag. field 4.46451
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Lz=3 S7=-2.5	0	0	0	0	0	-69.93798	0	0	0	0		-3.364251
		0	0	0	0	XXXX	-0.02054	0	0	0	0		+1.5554i
	1	0	<u>-1944.5436</u>	0	0	0	0	<u>-5500</u>	0	0	0		
xxx 0 0 0 0 31.84035 6.3211-4.7633 0 0 1	Lz=4 Sz=2.5	0.1647-4.92	0	0	0	0	0	17.89318	0	0	0		Selected row: 3
L2=4 0 0 -2459.6748 0 0 0 -3300 0 0 0 L2=4 0 0.1647-4.92 0 0 0 0 17.89318 0 0 0 L2=4 0 0.1647-4.92 0 0 0 0 17.89318 0 0 0 L2=4 0 0 -2668.8791 0 0 0 -240 0 0 0 -2668.8791 0 0 0 -2100 0 -2668.8791 0 0 0 -2668.8791 0 0 0 -2100 0 -2668.8791 0 0 0 -2100 0 -2668.8791 0 0 0 -2100 0 -2668.8791 0 0 0 1100 0 -2669.8791 0 0 0 0 27.8731 28.4807-6.3911 2 2 2001 2001 0 0 0 1100 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 <t< td=""><td></td><td>XXXX</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>31.84035</td><td><u>6.3211-4.763</u></td><td>0</td><td>0</td><td></td><td>Selected column: 9</td></t<>		XXXX	0	0	0	0	0	31.84035	<u>6.3211-4.763</u>	0	0		Selected column: 9
L2=4 0 0.1647-4.92 0 0 0 17.89318 0 0 0 2 0 XXX 0 0 0 0 XXX 24.76106 7.9956-6.0255 0 0 7 L2=4 0 0 0 2688.8791 0 0 0 1100 0 7 <th< td=""><td>1 - 1</td><td>0</td><td>0</td><td><u>-2459.6748</u></td><td>0</td><td>0</td><td>0</td><td>0</td><td><u>-3300</u></td><td>0</td><td>0</td><td></td><td>$L_z=4$ S_z=0.5</td></th<>	1 - 1	0	0	<u>-2459.6748</u>	0	0	0	0	<u>-3300</u>	0	0		$L_z=4$ S _z =0.5
0 xox 0 0 0 xox 24.76106 7.9956-6.025i 0 0 7000 70	Sz=1.5	0	0.1647-4.92i	0	0	0	0	0	17.89318	0	0		
L2=4 0 0 0 0 -1100 0 0 L2=4 0 0 0.16474.92i 0 0 0 17.89318 0 0 0 xxx 0 0 0 xxx 17.8178 84807-6.391i L2=4 0 0 0 0 0 0 0 1100 1 L2=4 0 0 0 0 0 0 0 1100 1 L2=4 0 0 0 0 0 0 0 1100 1 S2=0.5 0 0 0 0 0 0 1 100 100 100 L2=4 0 0 0 0 0 0 0 255 10.60249 7.995 12=4 0 0 0 0 0 0 0 0 3 12=4 0 0 0 0 100 0 3 4 12=4 0 0 0 0 <td></td> <td>0</td> <td>XXXX</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td> <td>XXXX</td> <td>24.76106</td> <td>7.9956-6.025</td> <td>0</td> <td></td> <td>Zoom+ Zoom-</td>		0	XXXX	0	0	0	0	XXXX	24.76106	7.9956-6.025	0		Zoom+ Zoom-
1/2 - 1 0 0 0.1647-4.92i 0 0 0 0 17.89318 0 Sz = 0.5 0 0 2xxx 0 0 0 0 2xxx 17.68178 8.4807-6.391i - Lz =4 0 0 0 0 0 0 0 100 100 Lz =4 0 0 0 0 0 0 0 1100 100 Lz =4 0 0 0 0.1647-4.92i 0 0 0 0 1100 1100 Lz =4 0 0 0 0.1647-4.92i 0 0 0 2xxx 10.60249 7.9954 Lz =4 0 0 0 1944.5436 0 0 0 3x Lz =4 0 0 0 1647-4.92i 0 0 0 3x Lz =4 0 0 0 1647-4.92i 0 0 0 0 3x 0 0 0 0 0 0 0	1-=4	0	0	0	-2608.8791	0	0	0	0	<u>-1100</u>	0		
0 0 xxx 0 0 0 xxx 17.68178 8.4807-6.3911 Lz=4 0 0 0 -2459.6748 0 0 0 100 100 Lz=4 0 0 0 0.1647-4.92i 0 0 0 17.89318 7.995 0 0 0 0 0 0 0 3 1.60249 7.995 0 0 0 0 0 0 0 3 1.60249 7.995 1 0 0 0 0 0 0 0 3 1.60249 7.995 1 0 0 0 0 1.647-4.92i 0 0 0 3 1.60249 7.995 1 0 0 0.1647-4.92i 0 0 0 3 1.60249 1.612 1.612 1 1 1 1 1.612 1.612 0 0 0 1.612 1.612 1.612 1.612 1.612 1.612 1.612 1.612	Sz=0.5	0	0	0.1647-4.92	0	0	0	0	0	17.89318	0		
0 0 0 0 -2459.6748 0 0 0 1100 L2=4 0 0 0 0.1647-4.92 0 0 0 0 17.89318 0 0 0 0 0 0 0 0 7.9954 L2=4 0 0 0 0 0 0 3 L2=4 0 0 0 0 0 3 3 L2=4 0 0 0 0 0 3 3 0 0 0 0 1944.5436 0 0 0 3 L2=4 0 0 0 0.1647.4.92 0 0 0 3 3 0 0 0 0 0 0 0 3 3 3 0 0 0 0 0 0 0 3 3 3 0 0 0 0 0 0 3 3 3 3 3 3 3		0	0	XXXX	0	0	0	0	2000	17.68178	8.4807-6.391i		
1/2< 0 0 0 0.1647-4.92i 0 0 0 0 17.89318 5 0 0 0 2000 0 0 0 0 7.9951 Lz=4 0 0 0 0 0 0 0 0 33 Lz=4 0 0 0 0 -1944.5436 0 0 0 33 0 0 0 0 -1944.5436 0 0 0 33 Lz=4 0 0 0 0 -1944.5436 0 0 0 33 0 0 0 0 0.1647-4.92i 0 0 0 0 35 0 0 0 2000 0 0 0 35 35 35 0 0 0 2000 0 0 0 35 35 35 0 0 0 0 0 0 35 35 35 35 35 35 35 35	Lz=4 Sz=-0.5	0	0	0	0	-2459.6748	0	0	0	0	<u>1100</u>		
0 0 0 0 0 0 0 xxx 10.60249 7.995 0 0 0 0 -1944.5436 0 0 0 3 Lz=4 0 0 0 0 -1944.5436 0 0 0 3 0 0 0 0 0.1647-4.92i 0 0 0 0 17.1 0 0 0 0 xxx 0 0 0 2xxx 3.5 0 0 0 0 xxxx 0 0 0 3.5 -		0	0	0	0.1647-4.92i	0	0	0	0	0	17.89318		
0 0 0 0 -1944.5436 0 0 0 3 Lz=4 0 0 0 0.1647.4.92i 0 0 0 0 17.2 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 17.2 0 0 0 0 0 0 0 0 20.5 -		0	0	0	XXXX	0	0	0	0	XXXX	10.60249	7.995	
$S_{z}=-1.5 \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Lz=4 Sz=-1.5	0	0	0	0	0	-1944.5436	0	0	0	0	<u>3</u>	
		0	0	0	0	0.1647-4.92i	0	0	0	0	0	17.)	
		0	0	0	0	XXXX	0	0	0	0	XXXX	3.5	
		-			-			-	-				

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 (RusselSaunders 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

103

Energy Ei [K] 📼

78.941



ground state

-1-

- 0 000



-5000

-10000

around state

detailed information: eigenvalues eigenvectors scattering

parameters	s Hamiltonian	CEF view en	ergy levels sp	ectroscopy magneti	ic sus. Vinverse sus.	specific heat	entropy	description	
quantizati	on axis graph				1				
	×) ¥ : [1:1] ₽+		netic moment	observable transitions	J				
E [K]	ground term	energy levels	Energy Ei [K]	 expected va 	lues				
9000	66 Dy ⁺³	222	- 15309.618 - 15225.285 15190.392	$\begin{array}{l} < \! m_{tot} \! > \! = \! 0.0125 \mu_{\text{B}}, \\ < \! m_{tot} \! > \! = \! 0.0092 \mu_{\text{B}}, \\ < \! m_{tot} \! > \! = \! 0.0097 \mu_{\text{B}}, \end{array}$	α=70.18°, β=37.36° α=62.01°, β=37.50° α=76.19°, β=-142.0	8° m _t zoom n 8° m _t set visibl	avigation Q	200m scax 21.0x	
6000	el. config: 4J [*] base: LSL _z S _z > field: complex	2222	13404.520 13338.096 13296.119 13206.393	$< m_{tot} > = 0.2199 \mu_{B}, < m_{tot} > = 0.2318 \mu_{B}, < m_{tot} > = 0.1035 \mu_{B}, < m_{tot} > = 0.2330 \mu_{B},$	$\alpha = 90.11^{\circ}, \beta = 37.27^{\circ}$ $\alpha = 25.08^{\circ}, \beta = -149.3^{\circ}$ $\alpha = 76.05^{\circ}, \beta = -136.4^{\circ}$ $\alpha = 175.06^{\circ}, \beta = -141.5^{\circ}$	8° m, 7° m, 37° m,	highest 832	2.81K	
-		31213	10904.777 10899.265 10821.284 10790.730 10752.052	$\begin{array}{l} < m_{tot} > = 0.8837 \mu_{B}, \\ < m_{tot} > = 1.7580 \mu_{B}, \\ < m_{tot} > = 0.1903 \mu_{B}, \\ < m_{tot} > = 3.9449 \mu_{B}, \\ < m_{tot} > = 1.5303 \mu_{B}, \end{array}$	$\alpha = 57.25^{\circ}, \beta = 42.66^{\circ}$ $\alpha = 121.54^{\circ}, \beta = -131.$ $\alpha = 79.98^{\circ}, \beta = -157.6$ $\alpha = 9.28^{\circ}, \beta = 51.87^{\circ}$ $\alpha = 167.16^{\circ}, \beta = -132.$	64° m,	zero	PR 07/	
3000 —			7903.434 7862.731 7831.626 7811.140 7775.108	$\begin{array}{l} < m_{tal} > = 1.1623 \mu_{B'} \\ < m_{tal} > = 0.3745 \mu_{B'} \\ < m_{tal} > = 1.8601 \mu_{B'} \\ < m_{tal} > = 0.9397 \mu_{B'} \\ < m_{tal} > = 1.8067 \mu_{B'} \end{array}$	$\alpha = 65.69^{\circ}, \beta = 35.23^{\circ}$ $\alpha = 72.22^{\circ}, \beta = 34.44^{\circ}$ $\alpha = 73.72^{\circ}, \beta = 47.24^{\circ}$ $\alpha = 46.80^{\circ}, \beta = -140.4$ $\alpha = 30.42^{\circ}, \beta = -140.8$	5° m _t 5° m _t 6° m _{tet} = (-0.528, -0. 6° m _{tet} = (-0.710, -0.	.436, U.643) <m< td=""><td>close</td></m<>	close	
0 -	۴H	2122122	7748.849 7703.916	$< m_{tot}^{max} > = 5.8249 \mu_{B}^{\mu}, < m_{tot}^{max} > = 0.8979 \mu_{B},$	α=176.23°, β=24.72 α=99.71°, β=-142.7	2° m _{tot} =(0.348, 0. 1° m _{tot} =(-0.704, -0	160, -5.812) <m 0.536, -0.151) <m< td=""><td>i>=3.857 i_L>=0.594</td></m<></m 	i>=3.857 i _L >=0.594	
-3000		1222331	4318.820 4287.797 4257.018 4220.319 4189.529 4166.201 4133.469	$\begin{array}{l} < m_{tot} \! > \! = \! 7.2247 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 1.8250 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 2.5227 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 2.8936 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 0.1083 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 0.6378 \mu_{\text{B}}, \\ < m_{tot} \! > \! = \! 7.0934 \mu_{\text{B}}, \end{array}$	$\begin{array}{l} \alpha = 78.18^{\circ}, \ \beta = 38.07^{\circ} \\ \alpha = 81.73^{\circ}, \ \beta = 42.47^{\circ} \\ \alpha = 85.77^{\circ}, \ \beta = -137.6 \\ \alpha = 27.25^{\circ}, \ \beta = -139.1 \\ \alpha = 84.52^{\circ}, \ \beta = 159.22 \\ \alpha = 147.07^{\circ}, \ \beta = -154. \\ \alpha = 167.62^{\circ}, \ \beta = -139. \end{array}$	$\begin{array}{c} m_{tot} = (5.567, 4.1) \\ m_{tot} = (1.332, 1.1) \\ 4^{\circ} m_{tot} = (-1.859, -1) \\ 5^{\circ} m_{tot} = (-1.002, -0) \\ 2^{\circ} m_{tot} = (-0.101, 0) \\ 28^{\circ} m_{tot} = (-0.312, -0) \\ 84^{\circ} m_{tot} = (-1.162, -0) \\ \end{array}$	361, 1.480) <m< td=""> 219, 0.262) <m< td=""> .695, 0.186) <m< td=""> 0.867, 2.572) <m< td=""> 0.38, 0.010) <m< td=""> .150, -0.535) <m< td=""> .981, -6.929) <m< td=""></m<></m<></m<></m<></m<></m<></m<>	ι _L >=4.006 ι _L >=1.045 ι _L >=1.425 ι _L >=1.610 ι _L >=0.059 ι _L >=0.341 ι _L >=3.997	
			- 284.566 - 253.098 - 212.163	$< m_{tot} > = 7.9553 \mu_{B}, < m_{tot} > = 3.9509 \mu_{B}, < m_{tot} > = 0.2617 \mu_{B},$	α=89.22°, β=38.61° α=89.17°, β=-135.3 α=65.84°, β=-148.2	$m_{tot} = (6.216, 4.0)$ $m_{tot} = (-2.808, -2.0)$ $m_{tot} = (-0.203, -0.0)$	964, 0.109) <m .779, 0.057) <m .126, 0.107) <m< td=""><td>L>=3.995 L>=1.987 L>=0.135</td></m<></m </m 	L>=3.995 L>=1.987 L>=0.135	
4 0 0		5221122		$< m_{tot} > = 1.4844 \mu_{B},$ $< m_{tot} > = 8.6056 \mu_{B},$ $< m_{tot} > = 2.2529 \mu_{B},$ $< m_{tot} > = 4.7311 \mu_{B},$ $< m_{tot} > = 2.7815 \mu_{B},$	$\alpha = 72.89^{\circ}, \beta = -148.1^{\circ}$ $\alpha = 15.24^{\circ}, \beta = 38.45^{\circ}$ $\alpha = 159.48^{\circ}, \beta = 34.21^{\circ}$ $\alpha = 27.39^{\circ}, \beta = 39.19^{\circ}$ $\alpha = 155.55^{\circ}, \beta = -128.2^{\circ}$	$ \begin{array}{c} \mathbf{b}^{\circ} & \mathbf{m}_{tot} = (-1.205, -0.55, -0.$	1.748, 0.437) <m 407, 8.303) <m 444, -2.110) <m 376, 4.201) <m 1.898, -2.532) <m< td=""><td>L>=0.738 L>=4.308 L>=1.135 L>=2.350 L>=1.388</td></m<></m </m </m </m 	L>=0.738 L>=4.308 L>=1.135 L>=2.350 L>=1.388	
3+	ground state	235112	0.000						

eigenfunction[4] = -0.0001-0.0001i|+6.0,+1> +0.1317+0.0104i|+6.0,0> -0.0002-0.0003i|+5.0,+2> +0.3699+0.0291i|+5.0,+1> -0.0001+0.0001i|+5.0,0> +0.4299+0.0338i|+4.0,+2> -0.0002+0.0002i|+4.0,+1> +0.0357+0.0028i|+4.0 EIGENVALUE:E[4] = -9381.0079

eigenfunction[5] = +0.3771|+6.0,+2> +0.0001-0.0001i|+6.0,+1> +0.0073|+6.0,-2> +0.0002-0.0002i|+5.0,+2> +0.0533|+5.0,-1> +0.0001+0.0001i|+4.0,+1> +0.1566|+4.0,0> +0.0001+0.0001i|+3.0,+2> +0.2365|+3.0,+1> +0.1803|+2 EIGENVALUE:E[5] = -9381.0035

4

eigenfunction[6] = +0.0003-0.0008i|+6.0,+2> +0.011+0.0266i|+6.0,+1> -0.0001-0.0001i|+6.0,0> -0.0292+0.0121i|+6.0,-1> +0.0191+0.0462i|+5.0,+2> -0.0004-0.0001i|+5.0,+1> -0.1194+0.0494i|+5.0,0> +-0.0001i|+5.0,-1> +0. 002i|-2.0,-2> +0.0058+0.0139i|-3.0,+2> -0.0001|-3.0,+1> -0.0154+0.0064i|-3.0,0> +0.0001-0.0003i|-3.0,-1> +0.0111+0.0268i|-3.0,-2> -0.0075+0.0031i|-4.0,+1> +0.0001-0.0002i|-4.0,0> +0.0123+0.0297i|-4.0,-1> -0.0003-0. EIGENVALUE: E[6] = -9377.8201

eigenfunction[7] = -0.0001-0.0002i|+6.0,+2> +0.2029+0.0734i|+6.0,+1> +0.0001-0.0001i|+6.0,0> +0.0014-0.004i|+6.0,-1> +0.3526+0.1276i|+5.0,+2> +0.0004-0.0002i|+5.0,+1> +0.0059-0.0162i|+5.0,0> +0.0021+0.0008i|+5.0,-+0.0001-0.0001i|-3.0,+1> +0.0008-0.0021i|-3.0,0> -0.0002-0.0005i|-3.0,-1> +0.2044+0.074i|-3.0,-2> +0.0004-0.001i|-4.0,+1> -0.0001-0.0003i|-4.0,0> +0.2269+0.0821i|-4.0,-1> +0.0005-0.0002i|-4.0,-2> +0.0001-0.0003i|-5 EIGENVALUE:E[7] = -9377.8201

eigenfunction[8] = -0.556+0.0001i|+6.0,+2> +0.0001-0.0001i|+6.0,+1> -0.0102|+6.0,-2> +0.0001-0.0001i|+5.0,+2> -0.0705|+5.0,-1> -0.2024|+4.0,0> -0.3028|+3.0,+1> -0.2307|+2.0,+2> -0.0001-0.0001i|+2.0,-1> -0.001|+2.0 EIGENVALUE:E[8] = -9377.7805

CEF VIEW 8 CEF POTENTIAL VISUALIZATION

RESULTS

 $\alpha_{\beta\gamma}$

periodic table

parameters

 $V_{2}^{-2} = 0$

 $V_{2}^{-1} = 0$

 $V_{2}^{0} = 0$

 $V_{2}^{1} = 0$

 $V_{2}^{2} = 0$

 $V_{4}^{4} = 0$

 $V_{4}^{-2} = 0$

 $V_{4}^{-1} = 0$

0

 $V_{4}^{0} = 94.858$

0

0 $V_4^3 =$

0

V4 = 474.29

0

0 V-4=

0 $V_{6}^{-3} = 0$

V-3=

V1=

 $V_{4}^{2} =$

V 6 =

V-5=

 $V_{6}^{-2} = 0$

 $V_{6}^{-1} = 0$

 $V_{6}^{1} = 0$

 $V_{6}^{2} = 0$

 $V_{6}^{3} = 0$

 $V_{6}^{5} = 0$

 $V_{6}^{6} = 0$

V6= 74.55

V₆⁰ = 3.55

CEF view is a sub-tab of result tabs and has without interactive CEF design. The CEF view sub-tab only shows potential defined



s



9 SPECTROSCOPY ABSORPTION SPECTRA SIMULATION OF FINE ELECTRONIC STRUCTURE

RESULTS

The absorption spectrum of calculated Fine Electronic Structure can be simulated with

potential visualizer

set range

CEF view

 \mathbf{G}

50

V

V

V V V 5, 5, 5, 5,

100

intensity vs wave number (1/cm)

150

200

Hamiltonian

periodic table

parameters

graph vie

1:1 2

100

75

50

25

insity (%)

O





RESULTS

periodic table

entropy S (J/K mol)

Hamiltonian

plot scale

1:1

19.0

14.3

9.5

4.8

0

0

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)

Result04

spectroscopy

energy levels

70

potential visualizer

 \cap

CEF view

set range

Bhe+2

el. config: 3d⁶ base: [LSL,S,>

field; complex

RIn 4

10

Atomic Matters v3.30 (24.04.16), 64-bit File Calculations Options Help

+2

Electronic configurati

+6

26 е

Iron

[Ar]3d⁶

L=2; S=2

Base

real

Parameters

 $B_{2}^{0} = -30 \text{ K}$

Result05

magnetic sus.

Entropy, sp Temperatu

0.02800

1.40000

2.80000

4.20000

5.60000

7.00000

8,40000

9.80000

11,20000

12.60000

14 00000

15.40000

16.80000

18.20000

140

temperature T(K)

CEE Parameters

B⁰ = -133.33 K

Spin-orbit constant $\lambda_{s=0} = -150 \text{ K}$

Magnetic field (static)

Bext=0T

to zero)

0.0859347

0.0000347

0.0051513

0.1090386

0.4226106

0.8567825

1.2746645

1.6021802

1.8224868

1.9474009

1,9978691

1.9947097

1.9552595

1.8929149

210

6.8575403

7.0658897

7.2565107

7,4285913

7.5827496

280

B³₄ = -3771 K

ground term: ⁵D

Hamiltonian matrix

3



⇒Fine electronic structure of ions, Spectrum simulations and all calculation settings \Rightarrow 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

- • ×



MAGNETIC SUSCEPTIBILITY 1 and INVERSE MAGNETIC SUSCEPTIBILITY

RESULTS

Electronic configu

+6

Iron

[Ar]3d⁶

L=2; S=2 ground term: ⁵D

Base

26 Fe

2 graphs of thermal variation of magnetic susceptibility for orthogonal directions of an inducing



Atomic Matters v3.30 (24.04.16), 64-bit - • × File Calculations Options Help 🔚 🗛 🕸 🗗 🖩 🎬 🔟 🎄 🖨 ? 🗵 🕞 🤊 🖻 म periodic table potential visualizer Result04 Result05 s ecific heat spectroscopy magnetic sus. inverse sus. parameters Hamiltonian CEF view energy levels 0 +2 +3 +4 directions of magnetic field B plot scale Peff(z) = 6.19352 #8 • V V V 1:1 set markers (+) set range $P_{eff}(x) = 5.81966 \ \mu_B$ +2 B||z-axis B||x-axis B||y-axis $P_{eff}(y) = 5.81951 \ \mu_B$ 310.0 ₂₆ **Fe**⁺² $\chi_{x,y,z}^{-1}(10^{-1}\,T/\mu_B)$ el. config: 3d6 $\alpha = 0.10^{-1}$; $\beta = 0.10^{-1}$ base: LSL, S, > field: complex 232.5 eptibility [B||x,y,z]



13 MAGNETOCALORIC EFFECT

ile Calculations Options Help

specific heat

11.25

7.5

3.75

detailed information

entropy

+ 1:1 set range



Calculation time: 0.9s

temp. range

ULT DATA

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 so 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 *.rtffiles.

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.

Pick results to save:

- IJJz> real Hamiltonian matrix
 IJJz> complex Hamiltonian matrix
- IL,S,Lz,Sz> real Hamiltonian matrix
- V aaa

Save options

save additional data (plot ranges, markers)

Physical Review Letters PRL 101, 217002-3 (2008)

Atomic Matters v3.36A (19.07.16), 64-bit File Calculations Options Help 💡 🔲 🎬 💹 🛃 🏤 🚾 🕞 🕞 File name: D:\---ATOMIC MATTERS---\W-Y-N-I-K-I\FU Description: Physical Review B 70, 134505 (2004) 🗟 🗐 📣 🚭 🗵 🚳 🖨 s Electronic configuration periodic table potential visu...er MCE calculations <J, Jz> real H...ix <J, Jz> compl...ix <L, S, Lz, Sz>r...ix <L, S, Lz, Sz>...an CEF view energy levels spectroscopy magnetic sus. inverse sus. specific heat entropy description 0 +3 +4 я² н н₂ - Black B I <u>U</u> Ē Tahoma +3 Results generated on 3-18-2016, at 08:26:51 AM (calculation time: 1.5s) for electronic configuration: 4f¹ 58 Ce Static calculation in [L,Lz,S,Sz> base with complex Hamiltonian Local symmetry: free/triclinic (complex) C_i C_1 Cerium Used CEF parameters: A₂⁰ = 0.0000000000 K/a₀², A₂¹ = 0.0000000000 K/a₀², A₂² = 186.1925133690 K/a₀², [Xe]4f1 A₄⁰ = 0.000000000 K/a₀⁴, A₄¹ = 0.000000000 K/a₀⁴, A₄² = 0.000000000 K/a₀⁴, A₄³ = 0.000000000 K/a₀⁴, A₄⁴ = L=3; S=1/2 0.000000000 K/a.4. ground term: ²F A₆⁰ = 0.000000000 K/a₀⁶, A₅¹ = 27.6681886983 K/a₀⁶, A₅² = 0.000000000 K/a₀⁶, A₅³ = 0.000000000 K/a₀⁶, A₅⁴ = $\alpha = -4.4 \cdot 10^{-2}$; $\beta = 4 \cdot 10^{-3}$ $0.000000000 \text{ K/a_0}^6$, $A_6^5 = 55.3363773966 \text{ K/a_0}^6$, $A_6^6 = 0.0000000000 \text{ K/a_0}^6$, $\gamma = -1 \cdot 10^{-3}$ Value of external magnetic field: 0.00 T Base Angle of external magnetic field (Z axis,XY plane): 0.00 deg. Angle of external magnetic field (X axis, Y axis): 0.00 deg. Hamiltonian matrix Spin-orbit cooeficient (lambda s-o): 920.00 K Please choose output directory: complex l real You can add/remove the informations in this area for this set o pper-right corner 🏭 Dysk lokalny (C:) of aplication and do not forget to save these changes Parameters Config.Msi dell +-CEF Parameters B2= -10.83227 K ÷... Intel ÷... JMatPro-v9-demo B4= 0.44314 K ÷... MiKTeX 2.9 $B_{4}^{4} = 0.88628 \text{ K}$ PerfLogs Program Files ÷... Program Files (x86) ÷... (values not shown are equal ProgramData ÷... to zero) Spin-orbit constant 🖃 c: [] $\lambda_{s=0} = 920 \text{ K}$ **1** [..] 2016-08-08 14:31 ----<DIR> Magnetic field (static) -B_{ext}=0T 2016-08-08 14:31 -a-g_spectro txt 58 $\alpha = 0.000$ $\beta = 0.000$ o spectro txt 58 2016-08-08 14:31 -a-g_entr txt 58 2016-08-08 14:31 -a--Cancel OK txt 66 2016-08-08 14:31 -a-g_spech 2016-08-08 14:31 -a-g_chi txt 85 g_invchi txt 91 2016-08-08 14:31 -a-d moment txt 59 2016-08-08 14:31 -a-d temp txt 16 2016-08-08 14:31 -a-g E txt 2016-08-08 14:31 -a--0 2016-08-08 14:31 -a-o_spc txt 12 531 o_chi_z txt 12 260 2016-08-08 14:31 -a-o_chi_x txt 12 260 2016-08-08 14:31 -a-o_chi_y 12 260 2016-08-08 14:31 -a-txt 16 343 2016-08-08 14:31 -a-txt o neu οE 6 729 2016-08-08 14:31 -a-txt description rtf 2 0 3 8 2016-08-08 14:31 -a--OK Cancel



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.

> File name: D:\---ATOMIC MATTERS---\W-Y-N-I-K-I\FULL -WY Description: A.L. Lima et al. Phys. Rev. B 72 (2005) 024403

> > |J,Jz>B=1T [110]

3, 3, 3

energy levels spect

rules of transition

20

output data

Hamiltonian

range E (K) 1:1 2 0.01 - 61.090 set 0

|J,Jz> B=0T

CEF view

10

Mean Field Approximation (atomic matters MFA) v0.48a (02.08.16), 32-bit

input data

parameters

- graph view -

100

75

50

25

0

transition data

(%)

load file

🐻 🗐 🕞 😂 🚳 🚭 🚾 🕟 😥 🧣

() Mean Field Approximation (atomic ma	atters M	FA) v0.48a (02.08.16), 3	82-bit		-					- ¤ ×	
File Tabs Help	96	🕽 🕤 🗄 File name:	D:\ATOMIC I	MATTERS\W-Y-N-I-K-	I/FULL -WYNIKI PRZE	ECZESANE NEW COM	NCEPTION OF REAL	DER 07-2016\Dy3+i	in DyAl2 [110]-A	L Lima et al_PhysRevB72	
	in met d	Description:	: A.L. Lima et al.	Phys. Rev. B 72 (2005)	024403						
molecular-field coefficient:	load file	load file [J,Jz> B=0T [J,Jz>B=IT [110]									
$ \begin{array}{c} \textbf{molecular-field coefficient:} \\ \textbf{n}_{mol} = \boxed{3.6} & 7/\mu_{\text{B}} & \bullet \\ \textbf{set temperature steps:} \\ \hline \textbf{ST} = \boxed{2} & \textbf{K} \\ \textbf{set number of temperature steps:} \\ \hline \textbf{S0} & \textbf{steps} \\ \hline \textbf{Temperature range for calculations:} \\ \textbf{T} = \boxed{1.0.100} \text{ K} \\ \hline \textbf{Stimated calculation time:} \\ \textbf{7.05} \\ \hline \textbf{W} \\ \textbf{automate calculation for MCE} \\ \textbf{set external magn. field increment:} \\ \hline \textbf{S0}^{*}_{\text{ext}} = \boxed{0.5} & \textbf{Tesla} \\ \textbf{set external magn. field increment:} \\ \hline \textbf{S0}^{*}_{\text{ext}} = \boxed{0.1.01} & \textbf{Tesla} \\ \textbf{set external magn. field inferction:} \\ \hline \textbf{w} = \underbrace{0^{\circ}}_{0} & \textbf{set ps} \\ \textbf{B}_{\text{ext}} = \boxed{0.1.01} & \textbf{Tesla} \\ \textbf{set external magn. field direction:} \\ \hline \textbf{w} = \underbrace{0^{\circ}}_{0} & \textbf{set ps} \\ \textbf{Stemated calculation time:} \\ \textbf{42.05} \\ \hline \textbf{10} \\ \hline \textbf{10} \end{array} $	load file parameter $V_{2}^{2} = 1$ for fail for the fai	JJJZ> ers Hamiltonian value unit D Ka0 ⁻² D Ka0 ⁻⁴ D Ka0 ⁻² D Ka0 ⁻⁶ D Ka	B=OT CEF view Shape: Resolution: rotate shape	(J.J2> B=IT [10] energy levels 2 - + Very high w 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	spectroscopy	magnetic sus.		specific heat	entropy	description choose color palette standard 111 max 20 -0 -0 -0 -3.5521 	
	- select c	convolution	5								
Mean Field Approximation (at a second sec	tomic m	natters MFA) v0.49A	(05.08.16),	64-bit						- 🗆 X	
File Tabs Help											
	MCE		Description	R. Sasaki, D. Miura	, A. Sakuma, Appl	I. Phys. Express 8	8 (2015) 043004	5.0 onu			
MFA calculation parameters		input data	output	data							
molecular-field coefficient:		load file [],Jz	>B=0T L,	S,LZ,OT L,S,LZ,	1T L,S,Lz,	0T [J,Jz>rea],Jz>ce	x IL,S,Lz,Sa	L,S,Lze	ex	
$n_{mol} = 250 T/\mu_B \bullet$		parameters H	Hamiltonian	CEF view	energy levels	spectrosco	py magnet	ic sus. inver	se sus.	specific heat	
$\delta T = 10$ K			Û	Tahoma	\$	Black	‡ B	I U R ²	н н2		
set number of temperature steps:		Results generated	on 5-27-201	16, at 05:14:20 P	M (calculation t	ime: 34.6s) fo	r electronic co	nfiguration: 4f	3		
60 steps		Static calculation in	1 L,Lz,S,Sz	> base with comp (complex) C i C	ilex Hamiltoniar	n					
T=[0600] K		Used CEF paramet	ers: $A_2^0 =$	0.0000000000 K/	a_0^2 , $A_2^1 = 0.0$	000000000 K/a	a_0^2 , $A_2^2 = 45$	0.0000000000	K/a0 ² ,		
Estimated calculation time:		$A_4^0 = 0.00000000$	100 K/a ₀ 4, A	$\lambda_4^1 = 0.00000000$	00 K/a ₀ ⁴ , A ₄ ²	= 0.00000000	00 K/a ₀ ⁴ , A ₄ ³	= 0.00000000	000 K/a ₀ 4, A	N4 ⁴ =	
5111 46.05		0.000000000 K/a _c) ⁴ ,			2		AF		. 1	
U	4 /	$A_6^0 = 0.000000000000000000000000000000000$	00 K/a ₀ °, A	16 ¹ = -45.000000	$1000 \text{ K/a}_0^\circ, A_6$	5 ⁴ = 0.0000000	0000 К/а ₀ °, А 6	6 ⁵⁶ = 0.000000	0000 K/a ₀ °,	A ₆ ⁺ =	
automatic calculation		Value of external n	nagnetic fiel	ld: 0.00 T	-, ng 0.000	1000000 N a0	1.				
energ set external magn, field increment:		Angle of external n	nagnetic fiel	d (Z axis,XY plan	a): 0.00 deg.						
$\delta B'_{ext} = 1$ Tesla		Spin-orbit cooeficie	ent (lambda	s-o): 430.00 K	0.00 deg.						
set number of increment steps: 5 steps		You can add/remov of aplication and do	ve the inforn o <mark>not f</mark> orget	nations in this are to save these cha	a for this set o anges	if result separe	etely. Use text	formating butt	ons in the u	pper-right corner	

File Tabs Help

IFA calculation par

set temperature step:

δτ= 2 κ

molecular-field coefficient:

n_{mel}= 3.6 T/µ_B ▼

set number of temperature steps:

Temperature range for calculations: T=[0..100] K Estimated calculation time: 7.0s

automate calculations for MCE set external magn. field increment:

 $\begin{array}{l} \mathbf{B}'_{ext} = [\mathbf{0}..1\mathbf{0}] \ \mathbf{Tesla} \\ \text{set external magn. field direction:} \\ \alpha = \boxed{\mathbf{0}} \qquad \mathbf{0} \qquad \mathbf{\beta} = \boxed{\mathbf{0}} \qquad \mathbf{0} \\ \text{Estimated calculation time:} \\ \mathbf{42.0s} \\ \hline \mathbf{0} \end{array}$

δB'ext= 0.5 Tesla set number of increment steps: 20 steps

50 steps



atomic matters MFA INPUT DATA calculation parameters verifications 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.

(b) Mean Field Approximation (atomic matters MFA) v0.48a (02.08.16), 32-bit

MCE D

2





File name: D:\---ATOMIC MATTERS---\ Description: A.L. Lima et al. Phys. Rev. E

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 $B_{ext} = 5T$.

File Tabs Help

🔊 🗏 🕒 🖨 🥘 🔗

A screenshot of the thermal evolution of Fine Electronic Structure calculated by Atomic Matters MFA for Nd³⁺ ions in Nd₂Fe₁₄B supermagnets.



- 🗆 X







Two screenshots of thermal dependencies of the anisotropy constants $K_i(T)$ calculated by Atomic Matters MFA for Er³⁺ ions in Er₂Fe₁₄B compound and Nd³⁺ ions in Nd₂Fe₁₄B compound, respectively.

input data

load file

eneroy (MF)

+

-

- plot scale

1:1

273

173.75

74.5

-24.75

-124

Y

5

G

Vq0



temp. range

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 $B_{ext}=0$.

reference data). 2 ... 3 ... 4 ... 5 ... 6 ... 7 ... 8 ... 9 ... 10 inv. sus. (MF) anisotropy (MF) spec. heat ... F) entropy (MF) set type of graph plot scale (T]/T (T] + \mathbf{f} 1:1 set range 10 7.5 specific heat c (J/K · mol) 2.5 3 6 9 12 0.00 Temperature T(K)

temp. range



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.

(b) Mean Field Approximation (atomic matters MFA) v0.48a (02.08.16), 32-bit

File name: D:\---ATOMIC MAT

Description: A.L. Lima et al. Ph



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 $B_{ext} = 10T$.



AUTOMATIC MULTIPLE CALCULATIONS for MCE investigations MAGNETIC MOMENT result tab atomic matters MFA

File Tabs Help



atomic matters MFA AUTOMATING MULTIPLE CALCULATIONS for MCE investigations MAGNETIC MOMENT result tab



detailed information

and AUTOMATION of multiple MFA CALCULATIONS

Entropy curves $S_{max}(T,B_{ext})$ 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,Bast) to demonstrate magnetocaloric effect parameter

Temperature T(K) _

set markers (+)

100

temp. range

Two MCE entropy screenshots for the automated Atomic Matters MFA calculations for Nd³⁺ ions in NdNi₅ 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.

plot scale

4.5

1.5

0

entropy change - AS(J/K mol)

+ 1:1

-



12

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.



File Tabs Help

molecular-field coefficient:

set temperature step:

δT= 2 K

n_{mol}= 3.6 T/µ₈ ▼

MCE

input data

...ns

specific heat



Two screenshots of simulated thermal dependencies of specific heat curves c(T,B_{evt}) for the same compound DyAl₂ under the influence of an external magnetic field applied along different directions. This is an example of automated Atomic Matters MFA calculations for Dy³⁺ ions in DyAl₂ 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 Nd³⁺ ions in NdNi₅. The screenshots show specific heat curves c(T,Bext) and specific heat change $D(T,B_{ext})$ 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.

specific heat change $\Delta c(J/K \cdot mol)$



12

set markers (+)

curve c(B=0)

C_{mag}(B_i)

select



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www.atomicmatters.eu

