

Describing the Fine Electronic Structure and Predicting Properties of Materials with ATOMIC MATTERS Computation System

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Abstract—We present the concept and scientific methods and algorithms of our computation system called ATOMIC MATTERS. This is the first presentation of the new computer package, that allows its user to describe physical properties of atomic localized electron systems subject to electromagnetic interactions. Our solution applies to situations where an unclosed electron $2p/3p/3d/4d/5d/4f/5f$ subshell interacts with an electrostatic potential of definable symmetry and external magnetic field. Our methods are based on Crystal Electric Field (CEF) approach, which takes into consideration the electrostatic ligands field as well as the magnetic Zeeman effect. The application allowed us to predict macroscopic properties of materials such as: Magnetic, spectral and calorimetric as a result of physical properties of their fine electronic structure. We emphasize the importance of symmetry of charge surroundings of atom/ion, spin-orbit interactions (spin-orbit coupling) and the use of complex number matrices in the definition of the Hamiltonian. Calculation methods, algorithms and convention recalculation tools collected in ATOMIC MATTERS were chosen to permit the prediction of magnetic and spectral properties of materials in isostructural series.

Keywords—Atomic matters, crystal electric field, spin-orbit coupling, localized states, electron subshell, fine electronic structure.

I. INTRODUCTION

MATERIALS with special magnetic properties are of great importance to our civilization. Even though theoretical Solid State Physics provides a great number of theoretical approaches to predict magnetic properties of a material, these selectively describe the individual, specific properties of certain classes of substances. The clearly visible trend to adopt particular methodological apparatus to describe the properties of each group of materials results in a large amount of newly created models describing the characteristic physical properties of a particular class of compounds in solid state. There is a widely accepted opinion that the electron structure is responsible for all magnetic properties of the substance, but the notion is given a different meaning in different theoretical approaches. This confusion became the motivation for creating software that is intended to predict the properties of solid compounds with localized electron states and to help create new materials with properties dedicated to specific applications. Our aim was to find and parameterize the most important interactions in atom/ion in ligand surroundings. Such parameterization, comes directly from CEF theory, allows to transfer the influence of local charge

surroundings between different ions. We decided to call our computation system ATOMIC MATTERS.

II. MAIN ASSUMPTIONS OF THE THEORETICAL APPROACH

We assume that:

- All $2p/3p/3d/4d/5d/4f/5f$ - ions have a structure of discrete electron states affecting the properties of the whole compound.
- Multi-electron systems $2pn, 3pn, 3dn, 4dn, 5dn, 4fn, 5fn$ are strongly correlated electron systems.
- A description of such systems is based on atomic physics, with atomic numbers S, L, J of the entire shell. This results in the space of $n=(2S+1)(2L+1)$ states.
- In a solid, an atom/ion interacts with the environment (Stark effect) – this interaction leads to the abolition of the degeneracy of states and is referred to as the CEF.
- Through modifications of the fine structure of electron states of the atom, the CEF determines the properties of an atom in a solid and corresponds to the properties of the whole crystal.
- The spin-orbit coupling makes an important contribution to the structure of states and must be taken into account in the calculations.
- Magnetic interactions, both internal-intra ionic and with the external field, lead to further abolishment of state degeneracy (Zeeman effect).

As a consequence of our assumptions:

- The open shell atom/ion is a strongly-correlated electronic system.
- This strongly-correlated electronic system is described, following the atomic physics, by quantum numbers S, L (and J - if J is a good quantum number) of the whole shell. The ground term/multiplet is determined by Hund's rules. Then we work in the space of $(2S+1)(2L+1)$ states.
- In a solid, the open shell atom experiences charge interactions from the surrounding charge distribution – these interactions are known as CEF or sometimes as zero field splitting (ZFS).
- Crystal-field interactions result in the fine (discrete) electronic structure of an atom in a solid, that largely determines properties of the whole compound in solid state.
- This fine electronic structure is very sensitive to the local symmetry. The symmetry of the local surrounding is reflected in the symmetry of the crystal-field (CEF) Hamiltonian,

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- The magnetic ordering is reflected in the symmetry breaking of the eigenfunctions of many-electron states.

III. THEORETICAL METHODS

Our theoretical approach is deeply rooted in atomic physics. It is based on methods first defined by H.A. Bethe [1] in 1929 and further developed by hundreds of scientists, the most famous of them are: B.G. Wybourne [2], A. Abragam, B. Bleaney [3], R.J. Elliot, K.W.H. Stevens [4], [5], M.T. Hutchings [6], J.S. Griffith [7], G. Racah, B.R. Judd, J. Mulak, Z. Gajek [8], R.J. Radwański [9], C. Rudowicz [10], D.J. Newman [11].

Taking into consideration the individual population of energy levels of the fine electronic structure at different temperatures enables one to define the temperature dependencies of such properties as: free energy, magnetic entropy, magnetic susceptibility (calculated for different orientations of elementary cell in relation to the direction of magnetic field vector), p, d or f -electronic contribution to specific heat, structure of discrete electron levels and the probability of the INS (Inelastic Neutron Scattering) transitions, magnetic anisotropy, spin and orbital contribution to angular momentum of open electron subshell and many more. We use the following CEF+Spin-Orbit+Zeeman Hamiltonian:

$$H_{LS} = H_{CEF} + H_{S-O} + H_{Zeeman} = \\ = \sum_n \sum_m B_n^m \hat{O}_n^m(L, L_z) + \lambda \mathbf{L} \cdot \mathbf{S} + \mu_B (\mathbf{L} + g_e \mathbf{S}) \cdot \mathbf{B}_{ext}$$

or

$$H_J = H_{CEF} + H_{Zeeman} = \sum_n \sum_m B_n^m \hat{O}_n^m(J, J_z) + g_L \mu_B \mathbf{J} \cdot \mathbf{B}_{ext}$$

where B_n^m are CEF parameters, O_n^m are Stevens operators, λ is the spin-orbit constant, g_e is the gyromagnetic electron factor, μ_B is the Bohr magneton and B_{ext} is the external magnetic field. The eigenvectors of the Hamiltonian are described according to the selected base of calculations by the total momentum quantum numbers $|J, J_z\rangle$ or spin and orbit quantum numbers $|L, S, L_z, S_z\rangle$.

The calculated eigenvectors and expected values define spin and orbital magnetic moments of paramagnetic ions. Using the commutation relations of the angular momentum operators, we obtain information about expected values of the projections of magnetic momentum of all electronic states [3]-[6], [9].

Taking into consideration the possibility of the thermal population of states we automatically obtain thermal evolution of the single ion properties of the compound. This technique is based on the equivalent operator theory [4] defined as the CEF widened by thermodynamic and analytical calculations defined as the supplement of the CEF theory by including thermodynamic and analytical calculations.

At a temperature of $T = 0$ K, only the ground state is

occupied. In this situation, the magnetic moment of the ion is exactly equal to the momentum of the ground state. At extremely low temperatures, it is possible to excite the system e.g. by magnetic interaction with low-energy neutrons (which is used in Inelastic Neutron Scattering Spectroscopy, INS). It should be remembered, however, that the observed transitions are excitations from the ground state.

When the temperature rises, the probability of occupying higher states increases according to the Boltzmann statistics. The number of ions with the energy E_i within a system at temperature T , is:

$$N_i = N \frac{\exp\left(-\frac{E_i(T)}{k_B T}\right)}{Z(T)}, \\ Z(T) = \text{Tr} \left(\exp\left(-\frac{\hat{H}}{k_B T}\right) \right) = \sum_i \exp\left(-\frac{E_i(T)}{k_B T}\right)$$

In the above expression, N denotes the total number of particles, and Z is the statistical sum of states (partition function). Knowing the statistical sum of the states, we can determine the Helmholtz free energy $F(T)$:

$$F(T) = -k_B T \ln Z(T)$$

which allows estimating the internal energy $U(T)$ of the system:

$$U(T) = F(T) - T \left(\frac{\partial F(T)}{\partial T} \right) = -k_B T \frac{\partial}{\partial T} \left(\frac{F(T)}{k_B T} \right)$$

The fine structure of states (E_i, Γ_i) allows determining the thermodynamic functions for the statistical group of N ions. The most sensible value for is $N=N_A \approx 6.022 \cdot 10^{23} \text{ mol}^{-1}$ (Avogadro constant).

In our methodology, calculating the magnetization amounts to summing the identically behaving magnetic moments of individual ions with an unclosed electron shell. Due to the fact that the open subshell ions are in the self-aligned molecular field, their magnetic moment changes with temperature. Bearing in mind that each eigenstate of the CEF Hamiltonian is related to its magnetic moment, the total moment of a strongly correlated electron system at a given temperature is the resultant moment of occupied states calculated with the inclusion of the Boltzmann weight:

$$m_f^\alpha(T) = \frac{g_L \mu_B}{Z} \sum_i \langle J_\alpha^i \rangle \exp\left(-\frac{E_i(T)}{k_B T}\right)$$

where α indexes directional components, i - numbers the Hamiltonian eigenstates, while $\langle J_\alpha^i \rangle$ represents the expected value of the total angular momentum along the α -axis in the i -th state. This approach provides a clear way to determine the components of the total magnetic moment of paramagnetic ions. The total magnetic moment of the ion consists of the

orbital and spin parts: $m_c = m_l + m_s$.

More details about calculation methods of our theoretical

approach are available on ATOMIC MATTERS website [12] in the 'Theory' section.

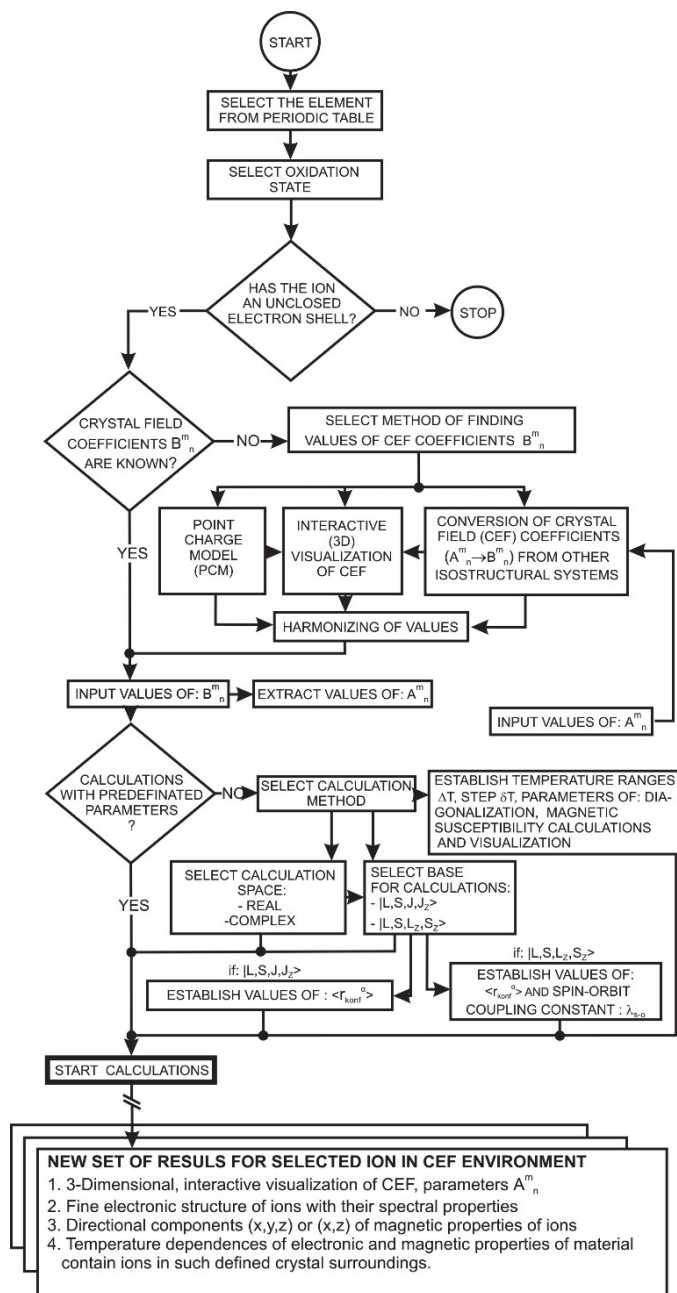


Fig. 1 ATOMIC MATTERS user decision tree

IV. SOFTWARE

The role of electron states for the magnetic, spectral and calorimetric properties of materials containing transition metals, rare earth metals, uranium group metals, is fundamental. However, there is much controversy in science when it comes to the selection of an adequate theoretical description of specific groups of chemical compounds in solid state.

Avoiding the doctrinal manifestoes, we just provide a tool for checking and comparing experimental results for actual materials with theoretical calculations. Our method relies on accurate quantum mechanical calculations and the formalism of operator equivalents (based on the Wigner-Eckart theorem) in Stevens formulation. ATOMIC MATTERS allows calculating the properties of materials and archiving them in a batch *.atma file, which represents a valuable piece of

knowledge about the magnetic, electronic and thermodynamic properties of a certain material. All *.atma files contain a well-developed information, in the form of graphs, diagrams, and texts that can be easily viewed, printed, etc.

Visual form of the result of calculations (including full 3D interactive potential visualization), intuitive method of interaction, fast access tools, and possibility of the comparison of data from different results allow the user to utilize the power of the application very effectively.

The user can decide to impose specific approximations on the calculations and decide for themselves which interactions are negligible and which are not. Fig. 1 shows the decision tree diagram for the user of ATOMIC MATTERS computer application.

Using the latest numerical methods for diagonalization of complex number Hamiltonian matrices [13], we are able to obtain a complete set of computational results (for realistic calculations) within a matter of seconds on typical PC hardware. Interaction with ATOMIC MATTERS involves generation of complete sets of input-output data, visualized in the form of charts, diagrams and 3D projections on sets of tabs with an intuitive, hierarchical structure. This allows for a quick verification of the impact of a specific interaction/parameter on the structure of the ion/atom and the effect on the macroscopic properties of the material. According to user decisions, ATOMIC MATTERS runs the calculations following the algorithm shown on Fig. 2.

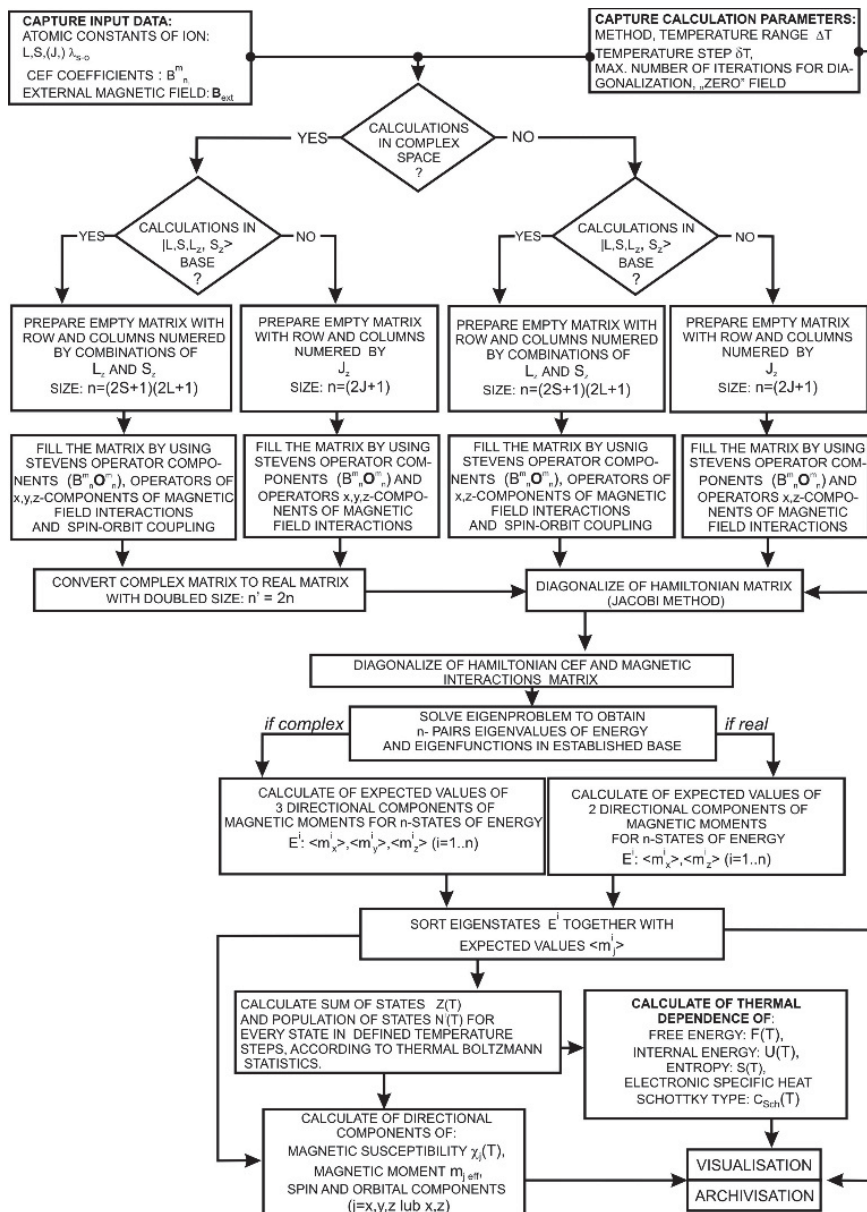


Fig. 2 ATOMIC MATTERS simple run algorithm

The calculations in the adopted basis ($|J, J_z\rangle$ or $|L, S, L_z, S_z\rangle$) result in the multiplet structure or term structure of multi-electron states. As a consequence, the following properties are predictable as temperature dependencies in a temperature range defined by the user:

- Electron entropy – related to the temperature filling of multi-electron states of the calculated electron structure of an ion or atom; $S_e(T)$
- Electron component of specific heat – related to the temperature filling of multi-electron states; $c_{Sch}(T)$
- Magnetic moment and magnetization, and its directional components; $m_i(B, T)$
- Magnetic susceptibility and its directional components - related to the temperature; $\chi_i(T)$
- Spin and orbital components of the total magnetic moment; $\langle \Gamma_i | \mathbf{m}_L | \Gamma_i \rangle$, $\langle \Gamma_i | \mathbf{m}_S | \Gamma_i \rangle$
- Spectroscopic observability of inter-state transitions; $\langle \Gamma_i | J_- | \Gamma_j \rangle$, $\langle \Gamma_i | J_+ | \Gamma_j \rangle$, $\langle \Gamma_i | J_z | \Gamma_j \rangle$ or $\langle \Gamma_i | L_- | \Gamma_j \rangle$, $\langle \Gamma_i | L_+ | \Gamma_j \rangle$, $\langle \Gamma_i | L_z | \Gamma_j \rangle$, $\langle \Gamma_i | S_- | \Gamma_j \rangle$, $\langle \Gamma_i | S_+ | \Gamma_j \rangle$, $\langle \Gamma_i | S_z | \Gamma_j \rangle$.

V. RESULTS

This is a first presentation of ATOMIC MATTERS algorithms, calculation methods and results. After a long time in development we were able to test our application in the area of crystals of Rare Earth (RE) 4f compounds, 3d/4d transition metal compounds and 5f metal compounds in different bases and under various limitations.

For the first announcement of our new computation system, we have decided to repeat some similar calculations from scientific publications of different authors. For testing purposes we performed calculations with ATOMIC MATTERS that successfully determined properties of several materials defined by its paramagnetic ions in real-world, solid compounds such as:

1. Ag^{2+} ion in Cs_2AgF_4 [13]
2. Ce^{3+} ion in $Ce_2Fe_{14}B$ [14]
3. Ce^{3+} ion in $CeAs$ [15]
4. Ce^{3+} ion in $CeBi$ [15]
5. Ce^{3+} ion in $CeFeAsO$ [16]
6. Ce^{3+} ion in $CeFeAsO_{0.84}F_{0.16}$ [16]
7. Ce^{3+} ion in $CeNi_{0.85}Cu_{0.15}Sn$ [17]
8. Ce^{3+} ion in CeP [17]
9. Ce^{3+} ion in $CeRh_{0.8}Pd_{0.2}Sb$ [17]
10. Ce^{3+} ion in $CeRh_{0.9}Pd_{0.1}Sb$ [17]
11. Ce^{3+} ion in $CeRu_2Ge_2$ [18]
12. Ce^{3+} ion in $CeRu_2Si_2$ [18]
13. Co^{3+} ion in $LaCoO_3$ [19]
14. Cu^{2+} ion in $Cu(C_2H_8N_2)_2Ni(CN)_4$ [20]
15. Dy^{3+} ion in Dy_2Fe_{17} [21]
16. Dy^{3+} ion in $DyCl_3$ [22]
17. Dy^{3+} ion in $DyNi_2$ [21]
18. Dy^{3+} ion in $DyNi_5$ [23]
19. Dy^{3+} ion in $DyRu_2Si_2$ [24]
20. Dy^{3+} ion in ethyl sulfate [25]
21. Dy^{3+} ion in $LaCl_3$ [25]
22. Dy^{3+} ion in Dy_2Co_{17} [21]
23. Er^{3+} ion in $Er_2Fe_{14}B$ [14]
24. Er^{3+} ion in Er_2Fe_{17} [21]
25. Er^{3+} ion in $ErAl_2$ [21]
26. Er^{3+} ion in $ErBa_2Cu_3O_7$ [26]
27. Er^{3+} ion in $ErCo_2$ [21]
28. Er^{3+} ion in $ErFe_2$ [21]
29. Er^{3+} ion in $ErNi_2$ [21]
30. Er^{3+} ion in $ErNi_2B_2C$ [27]
31. Er^{3+} ion in $ErNi_5$ [28]
32. Er^{3+} ion in $ErNiAl$ [29]
33. Er^{3+} ion in ErP [15]
34. Er^{3+} ion in $ErRh$ [15]
35. Er^{3+} ion in $ErRu_2Si_2$ [30]
36. Er^{3+} ion in ethyl sulfate [25]
37. Er^{3+} ion in $LaBr_3$ [15]
38. Er^{3+} ion in $LaCl_3$ [15]
39. Fe^{2+} ion in $FeBr_2$ [31]
40. Ho^{3+} ion in Ho_2Fe_{17} [21]
41. Ho^{3+} ion in $HoCo_2$ [21]
42. Ho^{3+} ion in $HoFe_2$ [21]
43. Ho^{3+} ion in $HoNi_2$ [21]
44. Ho^{3+} ion in $HoNi_5$ [23]
45. Ho^{3+} ion in HoP [15]
46. Ho^{3+} ion in $HoRh$ [15]
47. Ho^{3+} ion in $HoRu_2Si_2$ [24]
48. Mn^{3+} ion in $LaMnO_3$ [32]
49. Nd^{3+} ion in Nd_2Co_{17} [21]
50. Nd^{3+} ion in $NdCl_3$ [25]
51. Nd^{3+} ion in $NdCo_2$ [21]
52. Nd^{3+} ion in $NdFeAsO$ [33]
53. Nd^{3+} ion in NdN [15]
54. Nd^{3+} ion in $NdNi_2$ [21]
55. Nd^{3+} ion in $NdNi_5$ [23]
56. Nd^{3+} ion in NdP [15]
57. Nd^{3+} ion in $NdRu_2Si_2$ [24]
58. Nd^{3+} ion in NdS [15]
59. Nd^{3+} ion in $NdSe$ [15]
60. Ni^{2+} ion in NiO [34]
61. Np^{3+} ion in $NpGa_2$ [35]
62. Np^{3+} ion in $NpPd_2Al_3$ [36]
63. Pr^{3+} ion in ethyl sulfate [25]
64. Pr^{3+} ion in LaB_3 [15]
65. Pr^{3+} ion in $LaCl_3$ [25]
66. Pr^{3+} ion in $PrAg$ [37]
67. Pr^{3+} ion in $PrAs$ [37]
68. Pr^{3+} ion in $PrBi$ [37]
69. Pr^{3+} ion in $PrCl_3$ [15]
70. Pr^{3+} ion in $PrNi_2$ [21]
71. Pr^{3+} ion in $PrNi_2Si_2$ [38]
72. Pr^{3+} ion in $PrNi_5$ [23]
73. Pr^{3+} ion in PrP [37]
74. Pr^{3+} ion in PrS [37]
75. Pr^{3+} ion in $PrSb$ [37]
76. Pr^{3+} ion in $PrSe$ [37]
77. Pr^{3+} ion in $PrTe$ [37]
78. Pr^{3+} ion in $PrRu_2Si_2$ [39]
79. Sm^{3+} ion in ethyl sulfate [25]
80. Sm^{3+} ion in $Sm_2Fe_{17}C_{2.6}$ [40]

81. Sm^{3+} ion in $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ [40]
82. Sm^{3+} ion in $\text{SmBa}_2\text{Cu}_3\text{O}_7$ [41]
83. Sm^{3+} ion in SmNi_5 [42]
84. Sm^{3+} ion in SmP [15]
85. Sm^{3+} ion in SmSb [15]
86. Tb^{3+} ion in $\text{Tb}_2\text{Fe}_{17}$ [43]
87. Tb^{3+} ion in $\text{Tb}_2\text{Ti}_2\text{O}_7$ [44]
88. Tb^{3+} ion in TbCo_2 [21]
89. Tb^{3+} ion in TbFe_2 [21]
90. Tb^{3+} ion in TbNi_2 [21]
91. Tb^{3+} ion in TbNi_2Si_2 [38]
92. Tb^{3+} ion in TbNi_5 [23]
93. Tb^{3+} ion in TbP [15]
94. Tb^{3+} ion in TbPO_4 [15]
95. Tb^{3+} ion in TbRu_2Si_2 [24]
96. Tm^{3+} ion in ethyl sulfate [25]
97. Tm^{3+} ion in $\text{Tm}_2\text{Fe}_{17}$ [21]
98. Tm^{3+} ion in $\text{Tm}_{25}\text{Y}_{75}\text{Al}_2$ [15]
99. Tm^{3+} ion in TmBe_{13} [15]
100. Tm^{3+} ion in TmNi_2 [21]
101. Tm^{3+} ion in TmNi_5 [23]
102. Tm^{3+} ion in TmP [15]
103. Tm^{3+} ion in TmRu_2Si_2 [45]
104. Tm^{3+} ion in TmSb [15]
105. U^{3+} ion in UGa_2 [35]
106. U^{3+} ion in UPd_2Al_3 [46]
107. U^{4+} ion in URu_2Si_2 [47]
108. Yb^{3+} ion in YbP [15]
109. Yb^{3+} ion in YbRu_2Si_2 [45]
110. Yb^{3+} ion in YbCu_2Si_2 [48]

For all cases (1-110), we have obtained full agreement with results of author's calculations in the most common aspects mentioned in the papers [13]-[48]. We have successfully translated CEF parameters from different conventions (B^n_m , $A^{m_n, <1^n>}$, B_{mn} , B^k_q , etc.) by using internal convention calculator implemented in ATOMIC MATTERS. The extracted CEF parameters allowed us to repeat calculations according to ref. [13]-[48] with full agreement. After reproduction of the results from references, we have decided to perform similar calculations, with the same A^n_m CEF parameters for all cases above, with extended calculation base (from $(|J, J_z\rangle$ to $|L, S, L_z, S_z\rangle$) and extended Hamiltonian matrix elements (from real to complex field). The method of diagonalization of complex Hamiltonian matrices was based on 'A Simple Augmented Jacobi Method for Hermitian and Skew-Hermitian Matrices' from paper [49]. In agreement with author's suggestion we observe great increase of diagonalization speed after applying algorithms from [49].

All obtained results was converged with exactly-repeated author's calculations but many differences in directional, spin and orbital components of electronic states have been found. Starting data for all calculations were taken from the scientific papers, but all recognized crystal field parameters for compounds (1-110) can be used as a starting point for ATOMIC MATTERS calculations of new, structurally similar solid state compounds.

Each case of calculations needs a separate discussion, so we

have decided to provide easy access to all above results on our website – they are free to download as *.atma files [50], together with a free visualization program ATOMIC READER [51].

VI. CONCLUSION

Selected calculations, based on parameters taken from scientific publications (1-110) were performed using ATOMIC MATTERS. All cases of calculations provide some general conclusions:

In all cases, the $|L, S, L_z, S_z\rangle$ base is better for precise magnetism calculations and spectra recognition.

For some RE cases the $|J, J_z\rangle$ base is not adequate – especially for crystals containing Ce^{3+} and Sm^{3+} ions.

Calculations on complex number matrices always give more precise spectra information. Full, correct directional magnetic information are provided by calculations on complex number matrices only.

In general, the most commonly used calculation base $|J, J_z\rangle$ and real number matrix Hamiltonian should be chosen for calculation speed reasons only, because it offers approximate results with intermediate scientific value.

Working with ATOMIC MATTERS revealed its high usefulness. Visual form of the result of calculations, full 3D interactive CEF potential visualization, fast access tools for convention and unit recalculation, and possibility of the comparison of data from different results allow the user to utilize the power of the application very effectively. In conclusion we confirm that: ATOMIC MATTERS is the unique application combines a package of tools allowing the correctly describe of physical properties of atomic-like electron systems subjected to electromagnetic interactions typical of situations where an unclosed electron shell interacts with electrostatic potential of definable symmetry and external magnetic field.

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