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A new tool for the search of nuclides with properties suitable for nuclear solid state physics based on the Evaluated Nuclear Structure Data Files

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ABSTRACT

A software tool for the displaying of nuclear decay schemes, the calculation of angular γ emission anisotropies, and the automated search for appropriate decay cascade properties based on the Evaluated Nuclear Structure Data Files (ENSDF) was created and published for free download. After a short introduction of this tool, candidate nuclides for time differential perturbed γ–γ angular correlation (TDPAC) measurements are presented. These candidates are grouped according to their parent nuclides' half-life periods in groups for online, on-site, and off-site measurements. For all candidates angular correlation coefficients (also called *anisotropy values*) were computed and are shown alongside magnetic and quadrupole moments from the ENSDF database and other sources.

An extension of the presented software for the search of nuclides for Mössbauer spectroscopy, Nuclear Resonant Scattering, and other methods is easily possible.

1. Introduction

In the last decades methods belonging to nuclear solid state physics have significantly contributed to the understanding of condensed matter at the otherwise hardly accessible atomic scale. While e.g. the emission channeling method [1] allows for direct determination of impurity locations in the unit cells, it is possible to investigate magnetic fields and electric field gradients at probe nuclei applying Mössbauer [2] or time differential perturbed γ–γ angular correlation (TDPAC) spectroscopy [3], among others.

In these specific cases various different radioactive isotopes are applied as probes. This has rendered rare isotope separators, such as ISOLDE [4], invaluable tools where hundreds of radioactive isotopes are available for scientific experiments—many of them not available through neutron irradiation at conventional nuclear reactors. For certain studies the probe atoms should belong to specific chemical elements of interest or at least chemically similar ones. Additionally, each of these methods requires the used radioactive probe to have distinct properties. These are e.g. a particular decay type and Q value, an appropriate lifetime of the parent nuclide, suitable or electron and γ energies among others.

TDPAC may be considered the most ambitious among all of these methods, since it requires not only a γ–γ cascade, but also sufficiently large angular correlation coefficients and an appropriate lifetime of the intermediate level in conjunction with convenient magnetic dipole and/or electric quadrupole moments of this level such that these moments' interactions with the surrounding crystal fields yield interaction frequencies adequate for the spectrometers used.

Especially for the TDPAC method there has been a tremendous revival during the last years following the first successful proof-of-concept [5,6] and high-capacity [7] implementations of fully digital setups, which lead to an unprecedented versatility, thus opening exciting perspectives for this method at online isotope separators as well as research reactors. In this respect it is useful to have a close look at the isotopes used so far for TDPAC spectroscopy and examine to which extent the list of isotopes may be extended in the future considering that the better performance of modern spectrometers allows for improved on-site as well as on-line investigations now. This is especially important in order to increase the number of chemical elements that might be investigated.

The task of identifying useful isotopes for TDPAC experiments is solvable due to the availability of comprehensive high quality nuclear structure databases like ENSDF [8] and XUNDL [9]. The machine

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readable form, in which data is accessible by means of these databases, makes it possible to automate large parts of the search tasks thereby reducing the risk of missing promising candidates.

Existing universal tools for the search in these databases like e. g. *NuDat* [10] and the *Live Chart of Nuclides* [11] allow for the search of nuclides according to nuclear properties like Q values, γ energy, or half-life. However up to now, no solution existed for the search of nuclear decay cascades with properties suitable for TDPAC measurements.

In the following section we will introduce a software tool which was developed for the search and examination of decay cascades based on ENSDF data and which is published alongside this article. Additionally edited results of three relevant search runs grouped by the parent nuclides' half-life are presented including the most important parameters for TDPAC measurements.

2. Angular correlation coefficients

The calculation of angular correlation coefficients $A_{k_1k_2}$ is based on the orientation coefficients

$$B_\Lambda(\gamma_1) = [F_\Lambda(1,1,I_i,I) - 2\delta(\gamma_1)F_\Lambda(1,2,I_i,I) + \delta^2(\gamma_1)F_\Lambda(2,2,I_i,I)] \cdot [1+\delta^2(\gamma_1)]^{-1} \quad (1)$$

and the directional distribution coefficients

$$A_\Lambda(\gamma_2) = [F_\Lambda(1,1,I_f,I) + 2\delta(\gamma_2)F_\Lambda(1,2,I_f,I) + \delta^2(\gamma_2)F_\Lambda(2,2,I_f,I)] \cdot [1+\delta^2(\gamma_2)]^{-1} \quad (2)$$

as defined by Krane and Steffen (compare Eqs. (10) and (11) in Ref. [12]).

In these equations I is the intermediate level's spin while I_i and I_f are the initial and final levels' spins, respectively. $\delta(\gamma_1)$ is the mixing ratio of the first emitted γ photon originating from the transition $I_i \longrightarrow I$ whereas $\delta(\gamma_2)$ is the mixing ratio of the second γ photon from the transition $I \longrightarrow I_f$.

The F-coefficients are defined by Frauenfelder and Steffen (compare Eq. (96) in Ref. [3]) as

$$F(L,L',I',I) = [(2L+1)(2L'+1)(2I+1)(2k+1)]^{1/2} \cdot (-1)^{I'+I-1} \begin{pmatrix} L & L' & k \\ 1 & -1 & 0 \end{pmatrix} \begin{Bmatrix} L & L' & k \\ I & I & I' \end{Bmatrix} \quad (3)$$

including the Wigner 3-j and 6-j symbols.

Using Eqs. (1) and (2), the angular correlation coefficients $A_{k_1k_2}$ can be calculated:

$$A_{k_1k_2} = B_{k_1}(\gamma_1) \cdot A_{k_2}(\gamma_2) \quad (4)$$

Unfortunately, $A_{k_1k_2}$ is usually defined with $k_1 = k_2$ in literature (compare Eq. (98) in Ref. [3] or Eq. (14.31) in Ref. [13]). This simplification is based on the disappearance of the interference terms in unperturbed cases. Since this precondition is not fulfilled under the influence of quadrupole interactions the mixed terms are however relevant for solid state physics applications of TDPAC and are in fact often used in literature although not explicitly defined (e.g. Ref. [3], p. 1127). Our software uses mixing ratio and spin values from the ENSDF in order to calculate $B_\Lambda(\gamma_1)$ and $A_\Lambda(\gamma_2)$ for each possible decay cascade. It then uses these results to determine A_{22}, A_{24}, A_{42}, and A_{44} according to Eq. (4).

3. Software

A software tool named *Nuclei* was created for the systematic search of candidate nuclides as well as helping in setting up TDPAC spectrometers during measurements. This software is licensed under the GPL and freely available via SourceForge [14,15] in versions for Linux, MacOS X, and Windows.

It automatically downloads the most recent ENSDF database during its first startup. The downloaded files are then parsed to make relevant data accessible for automated processing.

Fig. 1 shows the main window of the user interface of *Nuclei*. In the left part a list of all daughter nuclides found in the ENSDF database is shown. After unfolding the sub-branch of a daughter nuclide all available parent nuclides and decays become visible. If one of these decays is selected, the appropriate decay scheme is shown in the program window's central part.

In this decay schemes two γ transitions can be selected by mouse clicks. Detailed data for selected transitions and the intermediate level is shown in the windows' right part. As soon as a decay cascade (i.e. two γ transitions with a common energy level) is selected, angular correlation coefficients are calculated according to Section 2 using libAkk [15] and shown at the bottom of the central part. libAkk computes the 3-j and 6-j symbols from Eq. (3) using implementations from the GNU Scientific Library [16]. Uncertainties from the ENSDF are propagated and shown as uncertainty in units of the least significant figure. Since possible correlations of the parameters' uncertainties are neglected, the resulting uncertainties can be considered as worst case estimates. In cases where no uncertainty value is available or the given value is "approximate" in the ENSDF results are prefixed by a tilde (~). If only upper or lower limits are given for mixing ratios the values are considered unknown for the calculation of angular correlation coefficients.

Because experimental values for A_λ and B_λ are usually not contained in the ENSDF records, these values are calculated using δ values from the ENSDF and Eqs. (1) and (2).

The tool bar contains buttons which allow for the export of decay schemes as PDF or SVG files including the highlighted decay path for easy utilization in publications. Additional buttons allow opening and closing both side panels containing decay selection as well as decay information. Four buttons are usable to adjust the zoom levels of decay schemes and photo peaks.

Fig. 2 shows the search dialog available by clicking the tool button showing binoculars in the main window. It allows defining limits for the parent nuclide's as well as intermediate level's half-life, magnetic dipole and/or electric quadrupole moments, angular correlation coefficients, γ intensities and the mass range of the search. For moments and angular correlation coefficients it is also selectable if checks should be skipped for entries with unknown values i.e. if entries containing unknown values should be added to the search results as if the unknown value matched the criteria or if they should be ignored. For these properties it is additionally selectable if all criteria must match or if it is sufficient if at least one matches. The results of a search run are afterwards shown instead of the nuclide list in the main window's left part.

For new TDPAC nuclides the interpretation of energy spectra can be rather cumbersome and – much worse during a measurement – time consuming. *Nuclei* is able to show photo peak spectra for each selected decay in order to simplify this work. Fig. 3 shows the spectrum for ^{169}Yb as an example. Compton scattering as well as pair production is ignored for these spectra to avoid detector specific behavior and keep it simple as the shown photo peaks are usually sufficient for the tuning of TDPAC setups.

If a γ cascade was selected the start and stop components are highlighted green and red respectively in the photo peak view. Other γ contributions are plotted stacked onto the selected transitions in order to provide an idea about intensity relations.

The energy resolution as well as linear or logarithmic plot styles can be changed in the tool bar. Additionally it is possible to change the font properties of decay schemes as well as the matching tolerance for decay data and adopted levels: As ENSDF data consists of results from many different experiments, data sets are not always perfectly consistent. Especially information concerning nuclear moments is often only available from the adopted