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1. Description

EPR simulator is a standalone application which demonstrates the basics of EPR spectroscopy. It is written in *MatLab*, using some functions of EasySpin package. *EPR simulator* requires MatLab Runtime shared libraries to be installed on your operating system.

2. Installation

To install the *EPR Simulator* run the following installer:

- EPRSimulator_v.3.0_setup.exe

The installer requires internet connection as the Runtime libraries must be downloaded from the web. Follow the instructions in the installation wizard.

3. Portable version

If you prefer not to install *EPR Simulator* on your system, you can use the portable version instead.

- EPRSimulator_v.3.0.exe

The portable version will run without installation, however you will need to install *MatLab Runtime* libraries, which are available online:

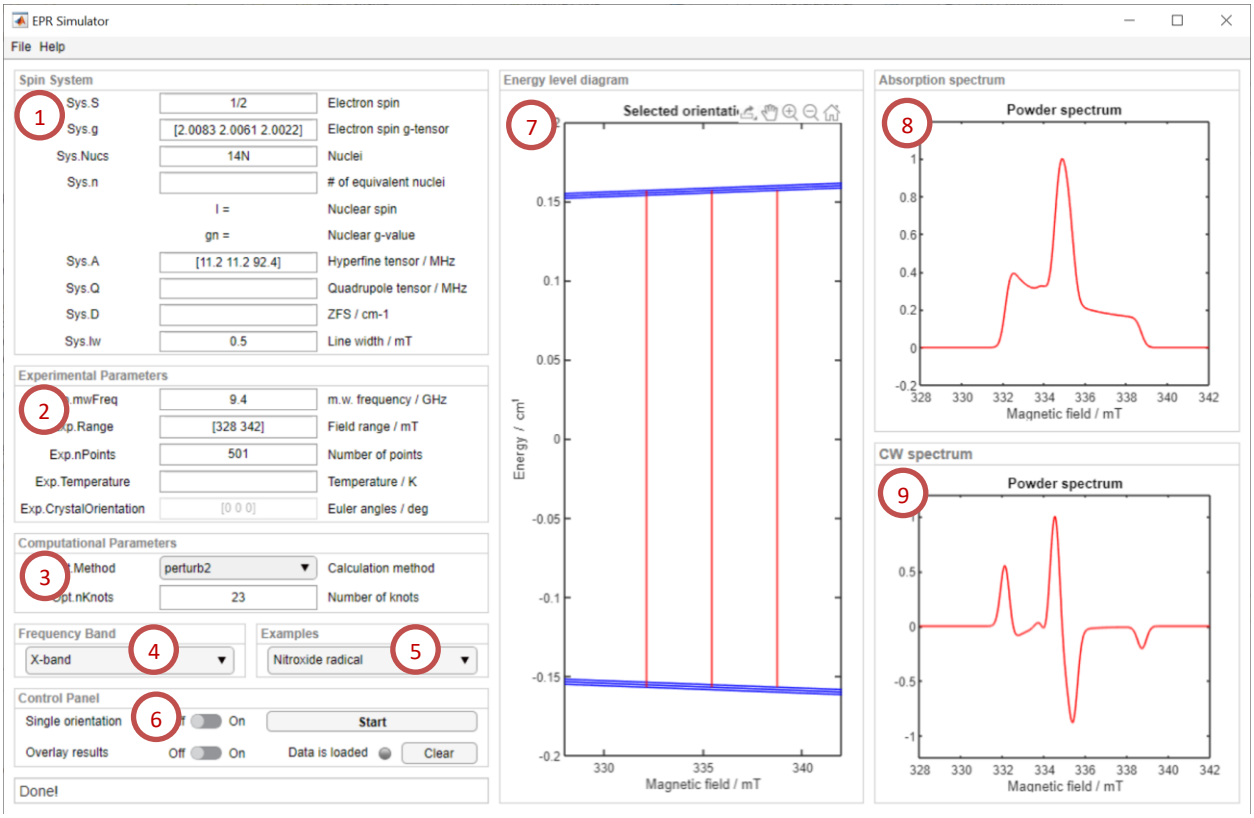
https://www.mathworks.com/products/compiler/matlab-runtime.html

The required version of Runtime libraries is specified in the readme file.

4. How to use the *EPR Simulator* package?

❖ Interface

There are several panels in the main window of *EPR Simulator*. On panels 1-3 you can set up the spin system, experimental and computational parameters. The labels used for different spin system elements are the same as those used in the EasySpin package. Panel 4 allows you to select the resonance frequency (note that it changes the experimental range = [Hmin Hmax], which is adjusted for only 'Nitroxide radical' example). Panel 5 provides a selection of examples; each option loads a set of preassigned parameters. With the 'Control Panel' (panel 6) you can run EPR spectra simulations, which will be plotted in panels 7-9. More details about each panel you will find below.



❖ Spin system parameters

EPR Simulator	EasySpin	Example	Description
Sys.S	Sys.S	0.5	Electronic spin quantum number
Sys.g	Sys.g	[2.01 2.004 2.001]	g-tensor
Sys.Nucs	Sys.Nucs	'14N'	Type of nucleus
Sys.n	Sys.nNucs	2	Number of equivalent nuclei
I	-	1	Nuclear spin quantum number
g_n	-	0.40376	Nuclear g-value
Sys.A	Sys.A	[10 10 90]	Hyperfine tensor / MHz
Sys.Q	Sys.Q	[Q η]	Quadrupole tensor (I>1/2) / MHz
Sys.D	Sys.D	[D E]	Zero-field splitting (S>1/2) / cm^{-1}
Sys.lw	Sys.lw	0.5	EPR linewidth / mT

❖ Experimental parameters

EPR Simulator	EasySpin	Example	Description
Exp.mwFreq	Exp.mwFreq	9.4	Resonance frequency / GHz
Exp.Range	Exp.Range	[320 340]	Field range / mT
Exp.nPoints	Exp.nPoints	501	Number of points in spectrum
Exp.Temperature	Exp.Temperature	298	Temperature / K
Exp.CrystalOrientation	Exp.CrystalOrientation	[0 90 0]	Orientation selection* / deg

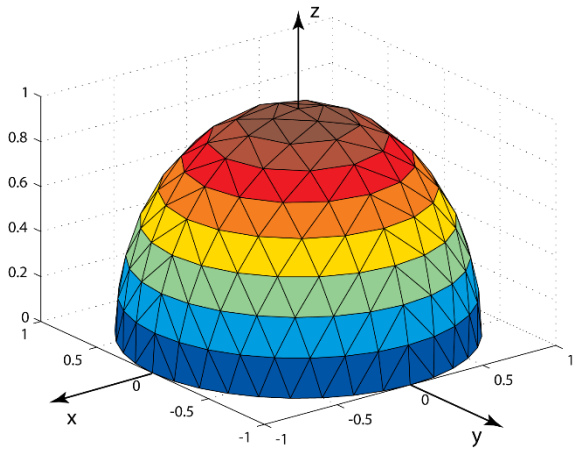
* there are different options for orientation selection, for example Exp.CrystalOrientation, for more details read EasySpin documentation.

Number of points (**nPoints**) has to be sufficient, that the spectral resolution, defined as dH = (Hmax-Hmin)/(nPoints-1), is smaller than the EPR linewidth.

❖ Computational parameters

EPR Simulator	EasySpin	Example	Description
Opt.Method	Opt.Method	9.4	Resonance frequency / GHz
Opt.nKnots	Opt.nKnots	31	Number of knots

The number of knots parameter (**nKnots**) defines the grid over the unit sphere used to sample orientation of the molecule in the magnetic field (laboratory frame). The input value defines a number of points on the segment of the sphere, where [φ θ] take values from 0 to π/2, each angle is .
For example, for nKnots = 10 (shown in a figure on the right) the θ step is 90/(nKnots-1), which equals 10 degrees. The corresponding φ angles are calculated in the same manner. The powder spectrum is an average over single orientation spectra of each knot on the grid.



❖ Examples

There are several basic examples (aka 'starting points') for quick parameter reset:

- ❖ 'Free electron' — spin system of a free electron: S=1/2, isotropic g-tensor;
- ❖ '1 Proton' — spin system of one proton: S=1/2; 1 nucleus (1H), isotropic g- and hyperfine tensors;
- ❖ '2 Protons' — spin system of two proton: S=1/2; 2 nuclei (1H), isotropic g- and hyperfine tensors;
- ❖ 'Nitroxide radical' — spin system of a nitroxide radical: S=1/2; 1 nucleus (14N), anisotropic g- and hyperfine tensors;
- ❖ 'Mn(III) ion' — spin system: S=2; 1 nucleus (55Mn), anisotropic g-tensor, ZFS;
- ❖ 'Fe(III) ion' — spin system: S=2.5; g=2, ZFS;

❖ Control panel

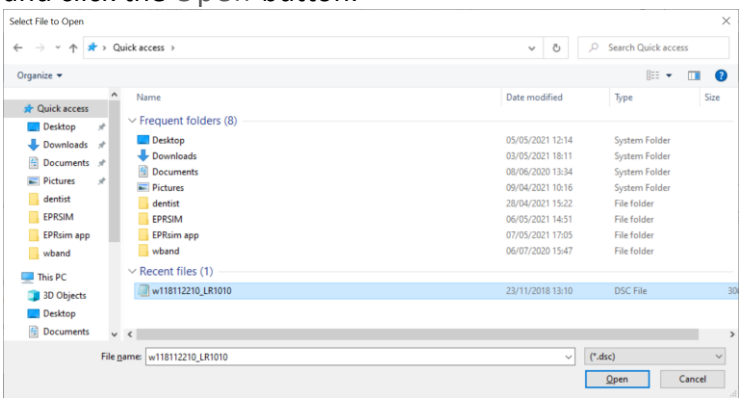
The 'Start' button runs the calculations and plots energy level diagram and simulated EPR spectra, both as the absorption and CW.
Note that the energy level diagram is calculated only for the orientation listed in the experimental panel, if the orientation is not given – it takes default values [0 0 0].

There are also two additional options that can be switched on and off:
'Single orientation' when selected – the program calculates spectrum of only one orientation as opposed to the whole powder spectrum. This could be used for simulating single crystal type EPR spectra.

'Overlay results' when selected this retains previously calculated spectra on the plot. This mode is useful for making figures with several single orientation spectra or when you wish to compare energy level diagram for different resonance frequencies or orientations.

❖ Loading experimental data

To load an experimental spectrum select the File -> Load menu. Select the desired *.dsc file and click the Open button.



❖ Saving parameters to a file

To save your parameters as a structure select the File -> Save menu. All the spin, experimental and computational parameters will be then saved to the specified *.mat file, which can be used to import those into *MatLab* environment for further calculations.