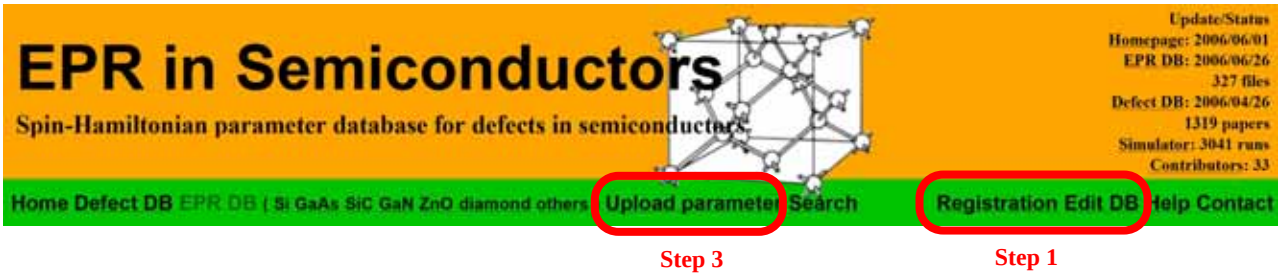
Appendix 1: How to upload new EPR data to "EPR in Semiconductors"

http://www.kc.tsukuba.ac.jp/div-media/epr/ → EPR in Semiconductors



Step 1.
Registration and Login

Finish registration (click *Registration* button) and login (click *Edit DB* button) on the web page.

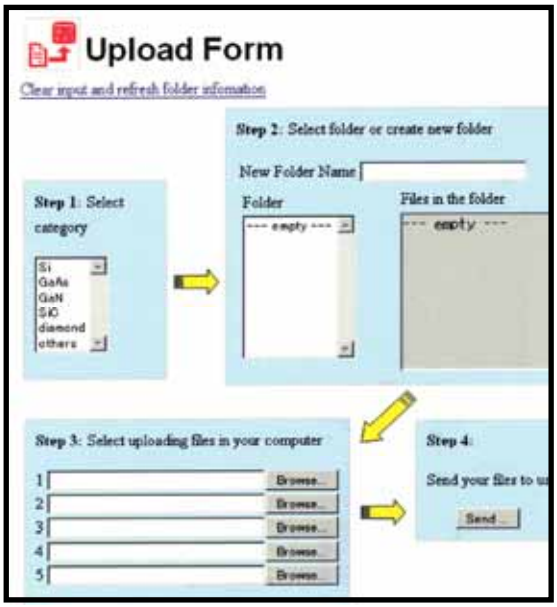
Step 2.
Prepare text files (page 2)

New EPR data [new Spin-Hamiltonian (SH) parameters of a defect] are formatted into a text file. Please see the next page for the format of the text file.

Step 3.
Upload

Upload the text files to the "EPR in Semiconductors" database using the Upload Form (Fig. 1).

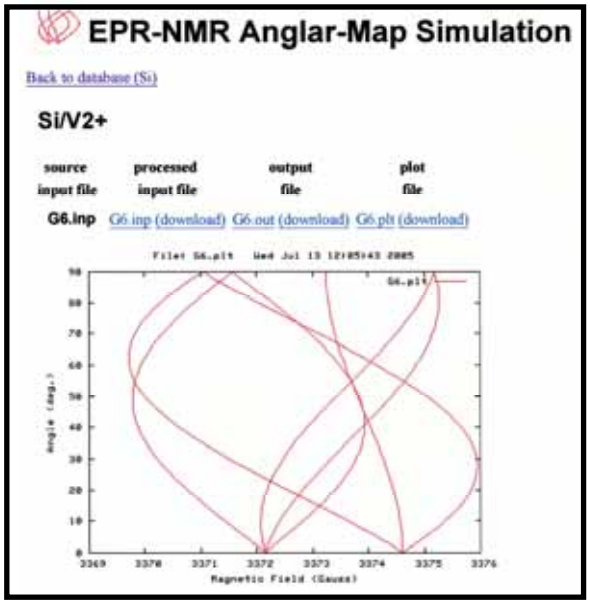
Fig. 1



Step 4.
Verification

Our server automatically executes an EPR-NMR© angular-map simulation using the uploaded files. Please check the calculated result shown on the web page (Fig. 2). If it is not consistent with that you expected, please follow the next step to revise the files.

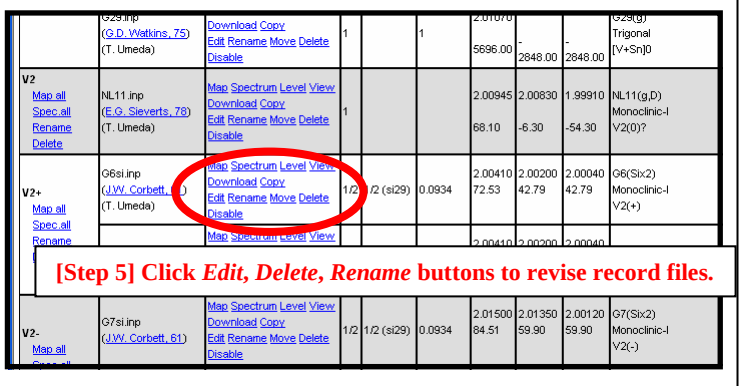
Fig. 2



Step 5.
Revision

If revisions are necessary for record files, please edit, rename or delete the files via the SH parameter list (Fig. 3). Please be careful that you cannot modify the records that were uploaded by other researchers.

Fig. 3



EPR data format (text file format)

Spin-Hamiltonian (SH) parameters of a defect are defined in a text file, as shown in below. Red color indicates the parts that we should replace by own data. The full details can be found on the web page: http://www.kc.tsukuba.ac.jp/div-media/epr/help/.

Example: ^{29}Si hyperfine structure of the famous Si G6 center)

```
ROADMAP, EPRFD, ECHO,
PRTPROPAR, EULER, ↲
PLOT=1, FREQ=9452.0, AUTONUC,
NSITE=12, NN=1↲
↲
Label:G6(Six2)↲
Author:T. Umeda↲
Reference:J.W. Corbett, G.D. Watkins,
Phys. Rev. Lett. 7, 314 (1961);G.D.
Watkins, J.W. Corbett, Phys. Rev.
138, A543 (1965).↲
Origin:V2(+)↲
Sample:low-resistivity p-Si irradiated
by 1.5-MeV electrons.↲
Symmetry:Monoclinic-I↲
Temperature:20K↲
Coordinate:x=[100],y=[011],z=[0-11]↲
RelativeIntensity:0.0934↲
OtherRemarks:Generation
rate=0.008defects/cm3 per
electron/cm2, strongly temperature-
dependent.↲
↲
0.5↲
si29↲
↲
2.0041    2.0004    2.0020↲      g tensor
-62.4     0         0↲
↲
72.53    42.79    42.79↲         29Si hyperfine
-55      0        0↲             tensor
↲
1, 1↲
↲
1   0   0↲
0   1   0↲
0   0   1↲
↲
-1  0   0↲
0   0  -1↲
0  -1   0↲
↲
1   0   0↲
0  -1   0↲
0   0  -1↲
↲
-1  0   0↲
0   0   1↲
0   1   0↲
↲
0          -0.707107   0.707107↲
0.707107   -0.5        -0.5↲
0.707107    0.5         0.5↲
↲
0           0.707107   -0.707107↲
-0.707107  -0.5        -0.5↲
-0.707107   0.5         0.5↲
↲
0          -0.707107   0.707107↲
-0.707107   0.5         0.5↲
-0.707107  -0.5        -0.5↲
↲
0           0.707107   -0.707107↲
0.707107    0.5         0.5↲
0.707107   -0.5        -0.5↲
↲
0           0.707107    0.707107↲
-0.707107  -0.5         0.5↲
0.707107   -0.5         0.5↲
↲
0          -0.707107   -0.707107↲
0.707107   -0.5         0.5↲
-0.707107  -0.5         0.5↲
↲
0          -0.707107   -0.707107↲
-0.707107   0.5        -0.5↲
0.707107    0.5        -0.5↲
↲
0           0.707107    0.707107↲
0.707107    0.5        -0.5↲
-0.707107   0.5        -0.5↲
↲
0,   0,   90,   0↲
0,   90,  2.0↲
↲
2↲
2,   3↲
1,   4↲
↲
2↲
2,   3↲
1,   4↲
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2,   3↲
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2,   3↲
1,   4↲
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2↲
2,   3↲
1,   4↲
```

(1) Command lines

This section describes EPR-NMR commands. No changes are necessary except FREQ, NSITE, and NN.

(2) Comment lines

These are just comments of the record and do not affect neither the definition of a spin system nor EPR-NMR simulations; but these are very useful for other users to understand this record.

(3) Electron spin (S)
Nuclear spins (I)

(4) SH parameters

Each SH tensor can be defined by either a matrix form or a set of three principal values and three Euler angles. This example adopts the latter format.

(5) Rotation matrices

In this example, 12 matrices (12 orientations of a defect) are set to express a diamond crystal of silicon. Other examples can be found on the web page for a cubic/NaCl crystal (24 sites), a Zinc-blend crystal (12 sites), and a hexagonal crystal (6 sites).

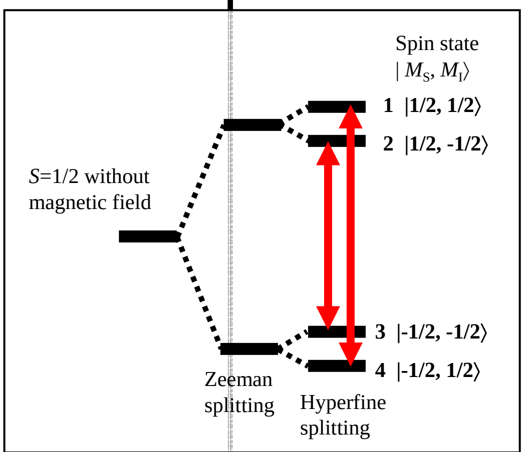
(6) Angular parameters

Define your magnetic-field rotation experiments. In this example, rotation axis = the *z* axis (polar angles θ=0°, ϕ=0°), the rotation starts from the *x* axis (θ=90°, ϕ=0°). Then, angular map can be calculated from 0° to 90° with 2.0° step, and you will see the calculated result in *Verification* (see step 4 in page 1).

(7) Transition table

When we execute the EPR-NMR© simulator, the given SH is numerically diagonalized, and finally we will obtain spin levels (=eigenvalues). To calculate an angular map or an EPR spectrum from the calculated levels, we have to specify which transition (=energy difference) we observe.

In this example, we set two EPR-allowed transitions (see below) for each orientation.



[Note] The format for the "EPR in Semiconductors" database is basically the same as used for a "ROADMAP" simulation of EPR-NMR©, which calculates an angular map of resonant fields with respect to a given crystal's rotation. Thus, EPR-NMR users may be already familiar to this format. We strongly encourage to reuse existing files in the database when one prepares new records. It will greatly reduce one's efforts.