XMGRACE INFO

The data files in this repository are stored as .xmgrace files. Grace is a free WYSIWYG 2D graph plotting tool, for Unix-like operating systems. You can find more info on <https://en.wikipedia.org/wiki/Grace_(plotting_tool)>.

To execute .xmgrace file, you simply need to run this command on any Unix-like operating system:

***xmgrace file.xmgrace***

The data associated with our work is stored in this format due to its compactness and an interested reader can reproduce any figure in our paper, with ease.

.xmgrace file is an ordinary text file and it can be open with any text editor. We advise Notepad++. Typically, the first set of lines have a form:

# Grace project file

#

@version 50123

@page size 792, 612

@page scroll 5%

@page inout 5%

@link page off

@map font 0 to "Times-Roman", "Times-Roman"

@map font 1 to "Times-Italic", "Times-Italic"

@map font 2 to "Times-Bold", "Times-Bold"

@map font 3 to "Times-BoldItalic", "Times-BoldItalic"

@map font 4 to "Helvetica", "Helvetica"

@map font 5 to "Helvetica-Oblique", "Helvetica-Oblique"

@map font 6 to "Helvetica-Bold", "Helvetica-Bold"

@map font 7 to "Helvetica-BoldOblique", "Helvetica-BoldOblique"

@map font 8 to "Courier", "Courier"

@map font 9 to "Courier-Oblique", "Courier-Oblique"

@map font 10 to "Courier-Bold", "Courier-Bold"

@map font 11 to "Courier-BoldOblique", "Courier-BoldOblique"

@map font 12 to "Symbol", "Symbol"

@map font 13 to "ZapfDingbats", "ZapfDingbats"

Lines starting with “@” are instruction for Grace plotting tool. The lines can be easily understood as simple figure settings, they set up x-y limits, colors, legends etc. What is important to understand in this file is how data information is stored.

Every graph in a figure has a label G0, G1, G2 … etc, every trace on a given graph has a label S0, S1, S2 … etc. For a standard x-y plot, only 1 graph and 1 trace exist, and info is stored after the line starting as @G0.S0, if the plot has multiple traces, next one will be at @G0.S1 etc.

If the figure has insets or different y-axis scaling (L-I-V figure for example), the first graph and its traces would be labeled as G0.S0, G0.S1, G0.S2 … etc, and the inset data would be stored in G1.S0, G1.S1, G1.S2 … etc.

In this repository, we stored the figure names in format figX\_description.xmgrace. X is the figure of interest, description is a short description about the the figures.

If Grace is unavailable and you wish to locate the data specifically, open any .xmgrace file in editor of your choice and navigate to the first occurrence of G0.S0 after which the data is stored in typical xy format. If the figure has multiple trace navigating to Gi.Sj would locate the data where Gi is the graph of interest and Sj is the trace of interest. Typically i=0 if there are no insets or dual axes on the graph, while Sj depends on how many trace are visible on the graph. Note that some figures as fig5\_doping.xmgrace does not fully follow this notation, thus for your convenience below is a table of all the traces for each figure individually:

|  |  |  |  |
| --- | --- | --- | --- |
| Figure name | Graph | Trace | Description |
| fig3\_simulogram.xmgrace | G0 | S0 | Material gain vs simulation number |
| fig4a\_Vwf\_3\_16\_81344.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (dark green) |
| S2 | The second state wavefunction (red) |
| S3 | The third state wavefunction (blue) |
| S4 | The fourth state wavefunction (green) |
| S5 | The fifth state wavefunction (orange) |
| S6 | The sixth state wavefunction (magenta) |
| S7 | The seventh state wavefunction (cyan) |
| S8 | Ground state wavefunction in the second period (dark green) |
| S9 | The second state wavefunction in the second period (red) |
| S10 | The third state wavefunction in the second period (blue) |
| S11 | The fourth state wavefunction in the second period (green) |
| S12 | The fifth state wavefunction in the second period (orange) |
| S13 | The sixth state wavefunction in the second period (magenta) |
| S14 | The seventh state wavefunction in the second period (cyan) |
| fig4b\_Vwf\_3\_24\_81341.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (dark green) |
| S2 | The second state wavefunction (red) |
| S3 | The third state wavefunction (blue) |
| S4 | The fourth state wavefunction (green) |
| S5 | The fifth state wavefunction (orange) |
| S6 | The sixth state wavefunction (magenta) |
| S7 | The seventh state wavefunction (cyan) |
| S8 | Ground state wavefunction in the second period (dark green) |
| S9 | The second state wavefunction in the second period (red) |
| S10 | The third state wavefunction in the second period (blue) |
| S11 | The fourth state wavefunction in the second period (green) |
| S12 | The fifth state wavefunction in the second period (orange) |
| S13 | The sixth state wavefunction in the second period (magenta) |
| S14 | The seventh state wavefunction in the second period (cyan) |
| fig4c\_Vwf\_3\_25\_79626.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (dark green) |
| S2 | The second state wavefunction (red) |
| S3 | The third state wavefunction (blue) |
| S4 | The fourth state wavefunction (green) |
| S5 | The fifth state wavefunction (orange) |
| S6 | The sixth state wavefunction (magenta) |
| S7 | The seventh state wavefunction (cyan) |
| S8 | Ground state wavefunction in the second period (dark green) |
| S9 | The second state wavefunction in the second period (red) |
| S10 | The third state wavefunction in the second period (blue) |
| S11 | The fourth state wavefunction in the second period (green) |
| S12 | The fifth state wavefunction in the second period (orange) |
| S13 | The sixth state wavefunction in the second period (magenta) |
| S14 | The seventh state wavefunction in the second period (cyan) |
| fig5\_doping.xmgrace | G0 | S6 | for (black) |
| S7 | for (red) |
| S8 | for (green) |
| S9 | for (blue) |
| S10 | for 4 (magenta) |
| S11 | for 4.5 (magenta) |
| G1 | S0 | for (black) |
| S1 | for (red) |
| S2 | for (green) |
| S3 | for (blue) |
| S4 | for 4 (magenta) |
| S5 | for 4.5 (magenta) |
| G2 | S0 – S11 | This graph has 12 traces in order for each point to have different color, S0-S5 refer to solid dots, S6-S11 to cross dots. |
| fig6a\_Vwf\_4\_18\_79421.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (dark green) |
| S2 | The second state wavefunction (purple) |
| S3 | The third state wavefunction (red) |
| S4 | The fourth state wavefunction (blue) |
| S5 | The fifth state wavefunction (orange) |
| S6 | The sixth state wavefunction (green) |
| S7 | The seventh state wavefunction (magent) |
| S8 | The eigth state wavefunction (cyan) |
| S9 | Ground state wavefunction in the second period (dark green) |
| S10 | The second state wavefunction in the second period (purple) |
| S11 | The third state wavefunction in the second period (red) |
| S12 | The fourth state wavefunction in the second period (blue) |
| S13 | The fifth state wavefunction in the second period (orange) |
| S14 | The sixth state wavefunction in the second period (green) |
| S15 | The seventh state wavefunction in the second period (magent) |
| S16 | The eigth state wavefunction in the second period (cyan) |
| fig6b\_Vwf\_4\_23\_103899.xmgrace | G0 | S0 | Band structure potential (black) |
| S1 | Ground state wavefunction (dark green) |
| S2 | The second state wavefunction (purple) |
| S3 | The third state wavefunction (red) |
| S4 | The fourth state wavefunction (blue) |
| S5 | The fifth state wavefunction (orange) |
| S6 | The sixth state wavefunction (green) |
| S7 | The seventh state wavefunction (magent) |
| S8 | The eigth state wavefunction (cyan) |
| S9 | Ground state wavefunction in the second period (dark green) |
| S10 | The second state wavefunction in the second period (purple) |
| S11 | The third state wavefunction in the second period (red) |
| S12 | The fourth state wavefunction in the second period (blue) |
| S13 | The fifth state wavefunction in the second period (orange) |
| S14 | The sixth state wavefunction in the second period (green) |
| S15 | The seventh state wavefunction in the second period (magent) |
| S16 | The eigth state wavefunction in the second period (cyan) |
| fig7\_injection\_barrier.xmgrace | G0 | S0 | with 9 monolayers (green) |
| S1 | with 10 monolayers (blue) |
| S2 | with 11 monolayers (magenta) |
| S3 | with 12 monolayers (red) |
| S4 | with 13 monolayers (cyan) |
| S5 | with 14 monolayers (orange) |
| S6 | with 15 monolayers (dark green) |
| G1 | S0 | with 9 monolayers (green) |
| S1 | with 10 monolayers (blue) |
| S2 | with 11 monolayers (magenta) |
| S3 | with 12 monolayers (red) |
| S4 | with 13 monolayers (cyan) |
| S5 | with 14 monolayers (orange) |
| S6 | with 15 monolayers (dark green) |
| G2 | S0 | with 9 monolayers (green) |
| S1 | with 10 monolayers (blue) |
| S2 | with 11 monolayers (magenta) |
| S3 | with 12 monolayers (red) |
| S4 | with 13 monolayers (cyan) |
| S5 | with 14 monolayers (orange) |
| S6 | with 15 monolayers (dark green) |
| fig8\_temp\_comparison.xmgrace | G0 | S0 | for 200K design (black) |
| S1 | for 210K design (red) |
| S2 | for 3\_16\_81344 design (blue) |
| S3 | for 3\_24\_81341 design (dark green) |
| S4 | for 3\_25\_79626 design (orange) |
| S5 | for 4\_22\_129641 design (magenta) |
| S6 | for 4\_23\_103899 design (cyan) |
| S7 | for 4\_18\_79421 design (green) |
| S8 | for 4\_23\_53103 design (purple) |
| G2 | S0-S8 | This graph is just a copy of the previous, zoomed around 220-250K, traces are identical to G1.S0-G1.S8 |
| fig8\_temp\_comparisonb.xmgrace | G0 | S0 | for 200K design (black) |
| S1 | for 210K design (red) |
| S2 | for 3\_16\_81344 design (blue) |
| S3 | for 3\_24\_81341 design (dark green) |
| S4 | for 3\_25\_79626 design (orange) |
| S5 | for 4\_22\_129641 design (magenta) |
| S6 | for 4\_23\_103899 design (cyan) |
| S7 | for 4\_18\_79421 design (green) |
| S8 | for 4\_23\_53103 design (purple) |
| G1 | S0-S8 | This graph is just a copy of the previous, zoomed around 220-250K, traces are identical to G1.S0-G1.S8 |

We apologize to the interested reader for the unorthodox storage of the data, but keep in mind that if we provided every individual x-y trace in a separate file, the repository would consist of very large number of files that would be hard to process. In this way, readers with access to Unix-like system can reproduce are figures with ease, while a Windows user would need to open the figX\_description.xmgrace files and navigate to the trace of interest with the help of the table above.

\*Note that in figure 5 the notation is slightly difference and first trace is G0.S6 instead G0.S0.

Kind regards,

The authors