Data information

This repository contains all data that corresponds to figures associated with our publication *“Acoustic band engineering in terahertz quantum-cascade lasers and arbitrary superlattices”*.

We have used Grace under Linux platform for generating figures in this work.

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)](https://en.wikipedia.org/wiki/Grace_%28plotting_tool%29). Grace also has open source support for Windows operating system <https://sourceforge.net/projects/qtgrace/> which uses .agr extension.

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

***xmgrace file.xmgrace***

or open the .***xmgrace*** file with qtgrace’s GUI (executable in the link <https://sourceforge.net/projects/qtgrace/> is located in bin/ directory, and no package installation is required).

As with many plotting tools, the data associated with the figures is directly available the .xmgrace files.

.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"

Lines starting with “@” are instructions 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 @target G0.S0, if the plot has multiple traces, next one will be at @target G0.S1 etc.

If the figure has insets or another y-axis. the first graph and its traces would be labeled as G0.S0, G0.S1, G0.S2 … etc, and the inset data would be targeted as G1.S0, G1.S1, G1.S2 … etc.

We decided not to provided data traces directly, as they can be easily found in .xmgrace files after searching @target GX.SY and understanding which trace in the figure corresponds to which target. Additionally, all our graphs can be recreated by simply using . xmgrace file with Grace in Linux or qtgrace in Windows.

The following table lists all . xmgrace figures in our paper and the corresponding GX.SY mapping of the traces represented in them.

|  |  |  |  |
| --- | --- | --- | --- |
| Filename | Graph | Trace | Description |
| Fig2\_Acoustic\_exp\_setup\_aa.xmgrace | G0(top graph) | S10 | $I(f)$ experimental data |
| G1 (bottom) | S0-S8 | Data lines that create the diamond representation of Brioullain zone folding |
| S10-20 | Data for marker dots in the graph – these values correspond to values we obtained numerically |
| Fig3\_Acoustic\_exp\_setup\_b.xmgrace | G0 (top) | S0 | $I(f)$ experimental data |
| G1-G2 (bottom) | S0-S9 | Similar to Fig2. |
| Fig4\_dfdn\_comp2.xmgrace | G0 (inset) | S0,S2, S3, S5, S6,S8, S9, S11 | These are traces for the 4 designs we analysed S0, S2 correspond to Hybrid structure, S3,S5 to LO phonon, S6, S8 to BTC structure, and S9, S11 to LO phonon structure in purple colour. Each group of traces illustrates data obtained numerically (full line) and by using averaged approximation (dotted lines)  |
| G1 (top) | S0, S4, S8, S12 | Offset from from the bulk approximation for four structures analysed in the figure. |
| G2(bottom) | S1, S5, S9, S13 | Offset from from the average approximation for four structures analysed in the figure. |
| Fig5\_dfdn\_exotic2.xmgrace | G0 | S0, S2, S3, S5, S6, S8 | These are traces for the 3 designs we analysed S0, S2 correspond to E structure, S3,S5 to F structure, S6, S8 to G structure. Each group of traces illustrates data obtained numerically (full line) and by using averaged approximation (dotted lines)  |
| G1 (top) | S0, S4, S8 | Offset from from the bulk approximation for three structures analysed in the figure. |
| G1 (top) | S0, S4, S8 | Offset from from the bulk approximation for three structures analysed in the figure. |
| Fig6\_dfdn\_mode\_manipulation. xmgrace | G0 -G5 | S0 | Each graph contains one data trace for the corresponding structure. G0 – Device A, G1 – Device B, G2 – Device C, G3 – Device D, G4 – Device E and G5 – Device H |
| Fig7\_dfdn\_mode\_manipulation\_altered. xmgrace | G0 -G5 | S0 | Each graph contains one data trace for the corresponding structure. G0 – Device D1, G1 – Device C1, G2 – Device C2, G3 – Device A1, G4 – Device I and G5 – Device J |
| Fig8\_fig-diffuse-profile \_altered. xmgrace | G0 (top) | S0, S1, S2, S4 | Data for offset from averaged approximation, S0 – Ld=0, S1 – Ld=2.8, S2 – Ld=4 and S4 – Ld=6.3 |
| G1 (middle) | S0, S1, S2, S4 | r.m.s of data presented in top graph |
| G2 (bottom) | S0, S1, S2, S4 | df/dn of data presented in graphs above. |
| Fig9\_Vwf\_hybrid.xmgrace | G0 | S0 | Bandstructure potenttial |
| S1 – S13 | Wavefunction traces in the first period |
| S2– S26 | Wavefunction traces in the second period |
| Fig10\_Hybrid\_transport\_M\_n30.xmgrace | G0 | S0 - S5 | g(K) data (left axis), each trace corresponds to different value of M = 0-5 meV |
| G1 | S0 - S5 | J(K) data (left axis), each trace corresponds to different value of M = 0-5 meV |
| G2(inset) | S0 - S5 | f(K) data (left axis), each trace corresponds to different value of M = 0-5 meV |
| Fig11\_Hybrid\_vs\_M\_stacked.xmgrace | G0 (a) | S0-S2 | g(M) data for n=1 (S0 trace), n=2 (S1 trace) and n=30 (S2 trace) |
| G1 (b) | S0-S2 | JNDR(M) data for n=1 (S0 trace), n=2 (S1 trace) and n=30 (S2 trace) |
| G2 (c) | S0-S2 | f(M) data for n=1 (S0 trace), n=2 (S1 trace) and n=30 (S2 trace) |
| G2 (d) | S0-S2 | Jdyn(M) data for n=1 (S0 trace), n=2 (S1 trace) and n=30 (S2 trace) |
| Fig12\_Hybrid\_vs\_pi\_stacked.xmgrace | G0 (a) | S0-S2 | g(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G1 (b) | S0-S2 | JNDR(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (c) | S0-S2 | f(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (d) | S0-S2 | Jdyn(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace)) |
| Fig13\_LO\_vs\_pi\_stacked.xmgrace | G0 (a) | S0-S2 | g(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G1 (b) | S0-S2 | JNDR(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (c) | S0-S2 | f(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (d) | S0-S2 | Jdyn(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace)) |
| Fig14\_BTC\_vs\_pi\_stacked\_stacked.xmgrace | G0 (a) | S0-S2 | g(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G1 (b) | S0-S2 | JNDR(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (c) | S0-S2 | f(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace) |
| G2 (d) | S0-S2 | Jdyn(n) data for M=1 meV (S0 trace), M=2 meV (S1 trace) and M=3 meV (S2 trace)) |

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, especially for wavefunction insets in Figure 9. In this way, readers can reproduce figures with ease, and get the corresponding figure data by accessing .xmgrace files in text editor.

Kind regards,

The authors