

IRGrace

A Package for making a grace file from data file

**User's guide, IRGrace_10.1(Release 23.09.2010)
Morteza Jamal**

Ghods city – Tehran-Iran

What is IRGrace?

IRGrace is a Package that helps you create a grace file from numerical data file

In order to use this Package the following public program packages must be installed :

- ▶ C-shell
- ▶ bc

Usually these public programs is available on Linux-systems.

This Package is the easiest way for making a grace file from data files and it can be very useful with xmgrace Package. It is sufficient use it for one time and you can understand why I say it is the easiest way for making a grace file.

Before using this package, I highly recommend provide a sheet and write in it informations about your frames and curves until you know what you want to plot and what informations you must to enter for your figs.

Copyright statement

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This Package is distributed in the hope that it will be useful.

Please let me know your ideas and send it to my email (m_jamal57@yahoo.com) until I can complete this package.

Installation guide

If you want to install this package please follow the following steps.

Copy “SRC_IRgrace.tar.gz” file in your computer.

```
tar -zxvf SRC_IRgrace.tar.gz
```

```
cd SRC_IRgrace
```

run “defbash_ir” program (type **defbash_ir** in Terminal Environment).

This program add PATH of IRGrace in the **.bashrc** file. So, you can call it in any where.

Call Package

To call this Package it is sufficient call **Ginf_grace_ir** (type **Ginf_grace_ir** in Terminal Environment).

What does IRGrace do?

This package help you create a STYLE file called **PersianGulf.info** and a grace file with name **PersianGulf.agr** .Therefore you can use this STYLE file for other figs that you would like to have the same style but, with different data. After making grace file, you can see it with selecting **Plotting → View agr file** menu (if you have installed xmgrace Package).

You can get the newest informations about xmgrace and download it at the Grace home page <http://plasma-gate.weizmann.ac.il/Grace/> .

For using this Package you must define ENVIRONMENT VARIABLE called IRGRACE_PATH in your **.bashrc** file. Program **Defbash_ir** do that for you.

Moreover this program help Wien2k users plot Density Of States (DOS) easily. For plotting DOS file, use this command (**Ginf_grace_ir -dos**) for non spin-polarized system and (**Ginf_grace_ir -dos -up/-dn**) for spin-polarized system. Then when you select **Plotting → Specify files and columns to plot** menu and define **PATH FILE FOR CURVE.....** , this program reads informations of case.int file and shows them and you are able to select column to plot , exactly the same as dosplot2_lapw program.

This Package creates and shows grace file when you make changes in **PersianGulf.info** by using **Ginf_grace_ir** program and it closes xmgrace program (when it shows grace file) after 10 seconds if you run **checkXM_ir** in another terminal or in background of your system by using **at** command.

With this program, you are able to enter data from different path. I highly recommend use this program for making a grace file from a data file.

The JPEG and PNG output will be available, when you select **Plotting → Save** menu, if additional libraries are installed when you install xmgrace. Those are:

The JPEG library <ftp://ftp.uu.net/graphics/jpeg/> , version 6.x.

The PNG library <http://www.libpng.org/pub/png/libpng.html> , version 0.96 or above

xmgrace permits quite complex typesetting on a per string basis. For more informations see userguide of xmgrace and “**control codes**” table in userguide of xmgrace.

In IRGrace Package, if you want to write a word as superscript or subscript for X-label or Y-label or Curve label type as follows:

`\s` for subscript , `\S` for superscript, and `\N` for normal type.

`V\szz` = V_{zz}

`V\Szz` = V^{zz}

`P\sxy\N-As` = $P_{xy}-A_s$

Moreover you are able to define different font (`\f<name of font>`) such as Symbol as follows (you can see **window** → **Font tool** in xmgrace menus):

`\f<Symbol>d` = δ

`\f<Symbol>D` = Δ

`\f<Symbol>D\f<>n\s d` = Δn_d `\f<>` = return to original font

`\f<x>` = switch to font named “x”

`\f<n>` = switch to font number n

`\f<>` = return to original font

`\R<x>` = switch to color named “x”

`\R<n>` = switch to color number n

`\R<>` = return to original color

`\z<x>` = zoom x times

`\z<>` = return to original zoom

`\r<x>` = rotate by x degrees

...

...

...

...

Main Menu

1- **Data**

2- **Style**

3- **X-axes**

4- **Y-axes**

5- **Font**

6- **Plotting**

7- **Add string**

8- **Quit**

1- Data Menu

1-1- Specify frame Menu

1-2- Specify curve

Define number of curve in each frame.

1-3- Specify files and columns to plot

Define PATH and name of file for getting data and columns to plot.

1-4- Quit

For exit.

Specify frame Menu

1-1-1- Specify number of frame (define number of frame)

1-1-2- Specify title (define title for each frame)

1-1-3- Specify subtitle (define subtitle for each frame)

1-1-4- Specify view position by hand (define view position of frame)

1-1-5- Specify view position automatically (define view position of frame)

1-1-6- Quit (for exit)

2- Style Menu

2-1- Specify line style

Define line style

2-2- Specify lines width

Define line width

2-3- Specify colors

Define line color

2-4- Specify symbols

Define symbol to show numerical data

2-5- Specify curve label

Define label for curve

2-6- Specify curve label position

Define view position for curve label

2-7- Quit

For exit

3- X-axes Menu

3-1- Specify label

Define label for X-axes

3-2- Specify scale

Define scale for X-axes

3-3- Specify major tick

Decide major tick for X-axes to be On/Off and In/Out and then define color and distance between major tick

3-4- Specify minor tick

Define number of minor tick between major tick and color for minor tick

3-5- Specify tick label

Decide tick label for X-axes to be On/Off and then define color for them

3-6- Quit

For exit

4- Y-axes Menu

It is the same as X-axes Menu

5- Font Menu

5-1- Specify font

Define type of font

5-2- Specify font size

Define size of font

5-3- Quit

For exit

6- Plotting Menu

6-1- Create

Creates grace file

6-2- View agr file

Shows grace file by using xmgrace

6-3- Save

Makes output (eps, png, jpeg) by using xmgrace

6-4- Quit

For exit

7- Add string

Define a string with special position, color, and degree

NOTE ABOUT PROGRAMS

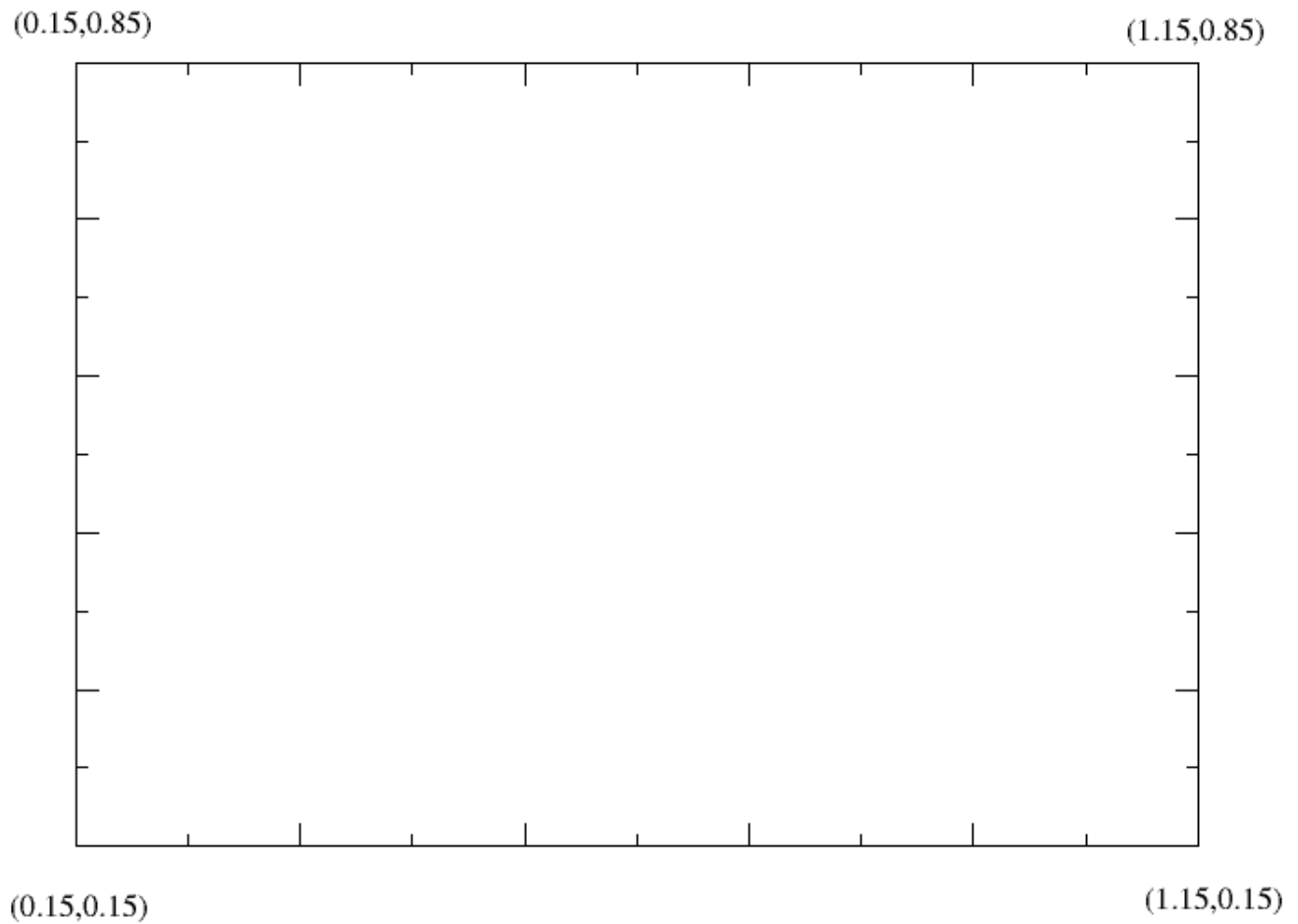
Ginf_grace_ir : This program gets informations and make STYLE file (**PersianGulf.info**) .

Cgrace_ir : This programs creates grace file (**PersianGulf.agr**) .

defbash_ir : Defines Environment Variable at the end of your **.bashrc** file.

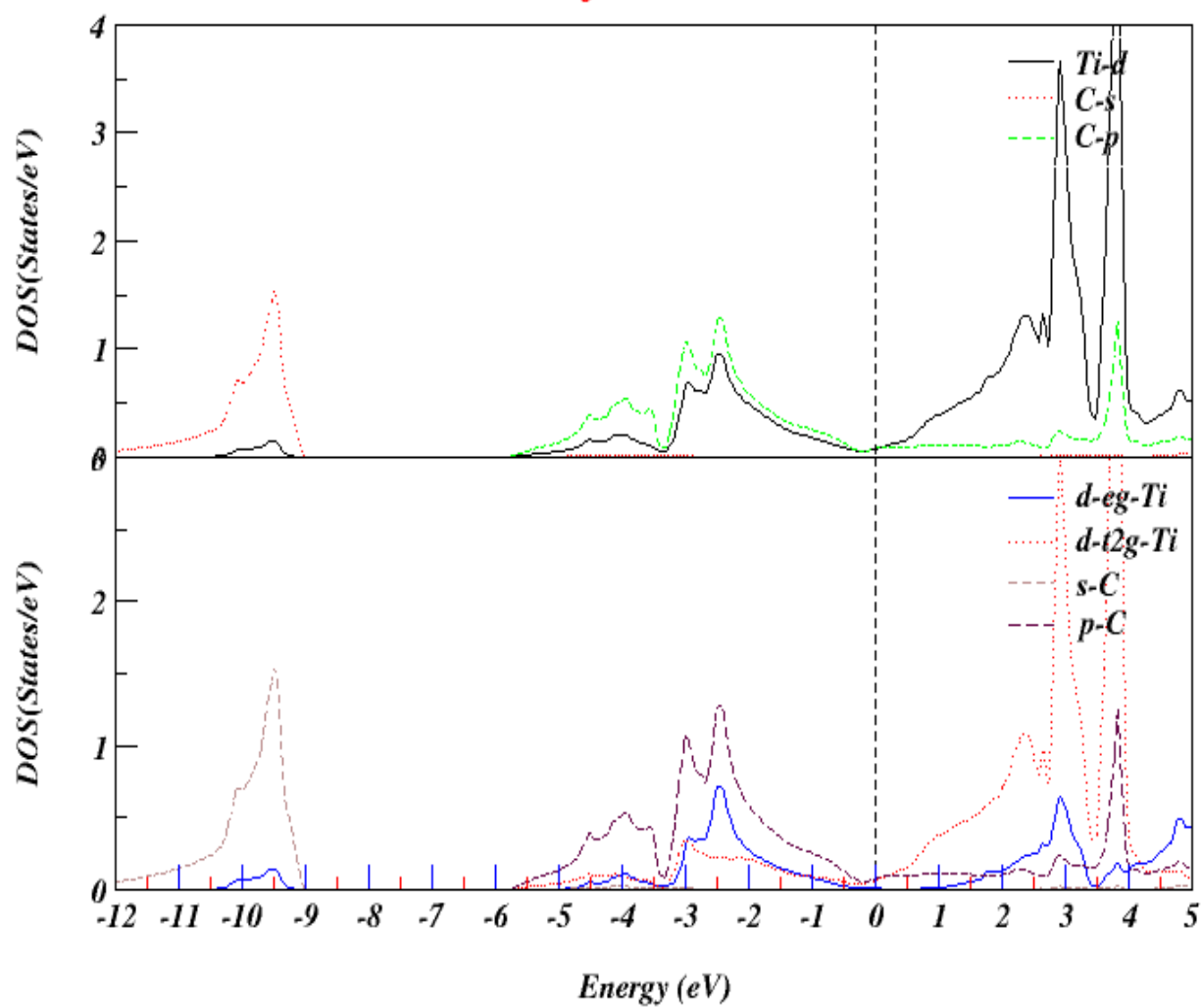
Deffun_ir: This program uses xmgrace program and with this program you are able to define a function for a curve.

Note: in this Package I have define the Xmgraxe window as follows:

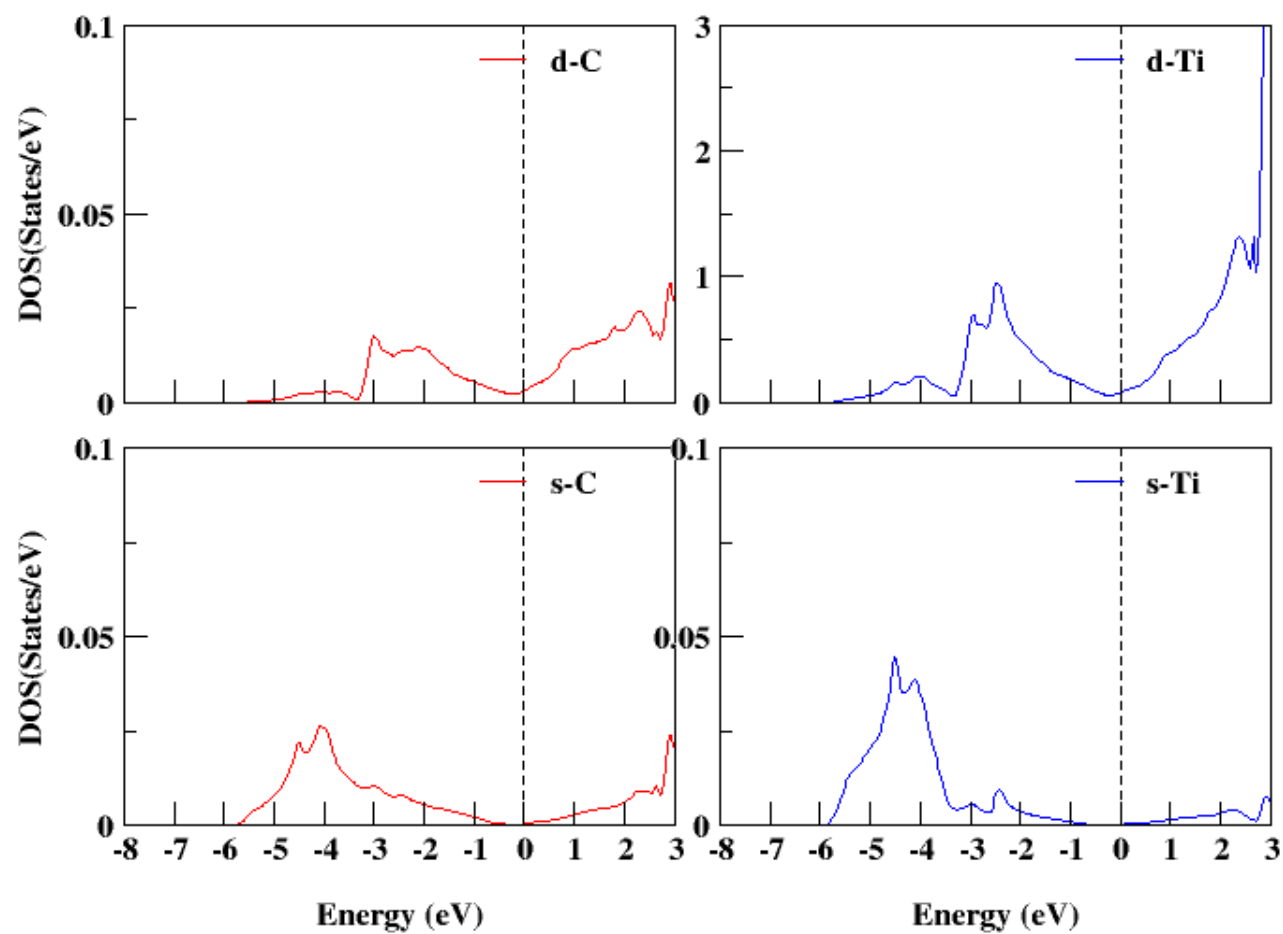


The following figs have been created by using this Package .

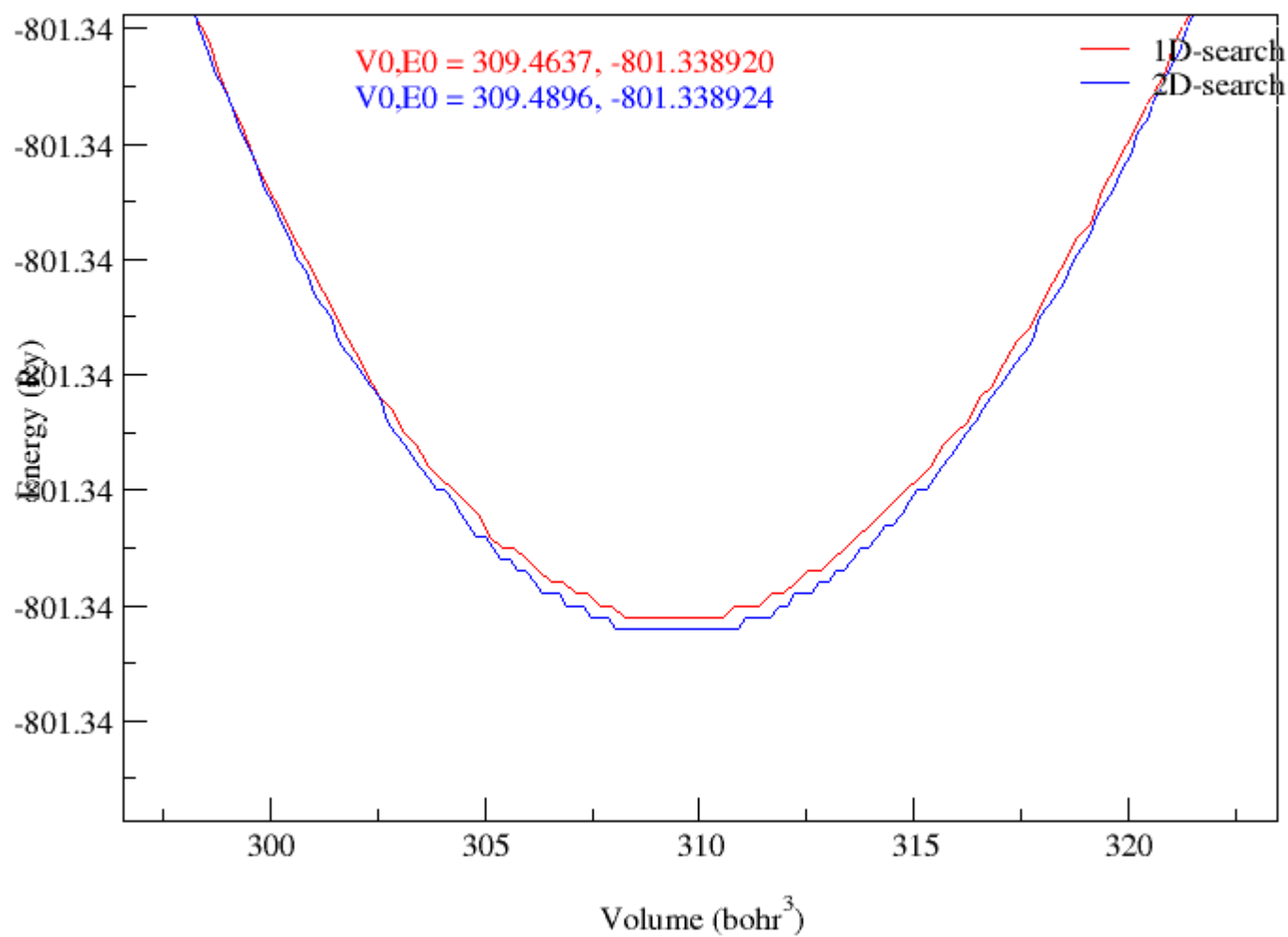
TiC-DOS
Data-from-Wien2k



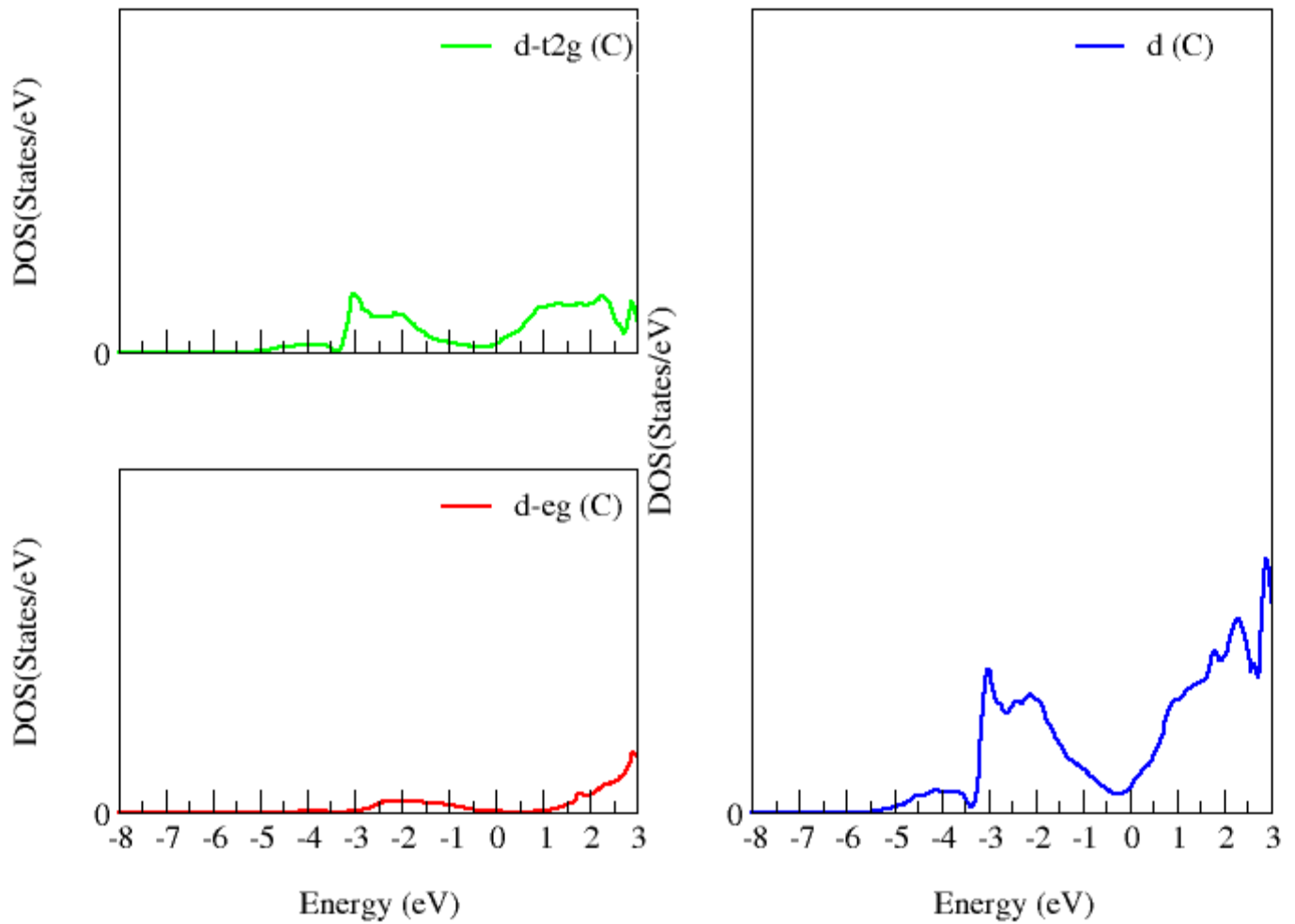
This plot has been created by using IRgrace and XMgrace



Equation Of State For hcp-Mg within GGA13



T_c



Have a nice day.....
Morteza Jamal