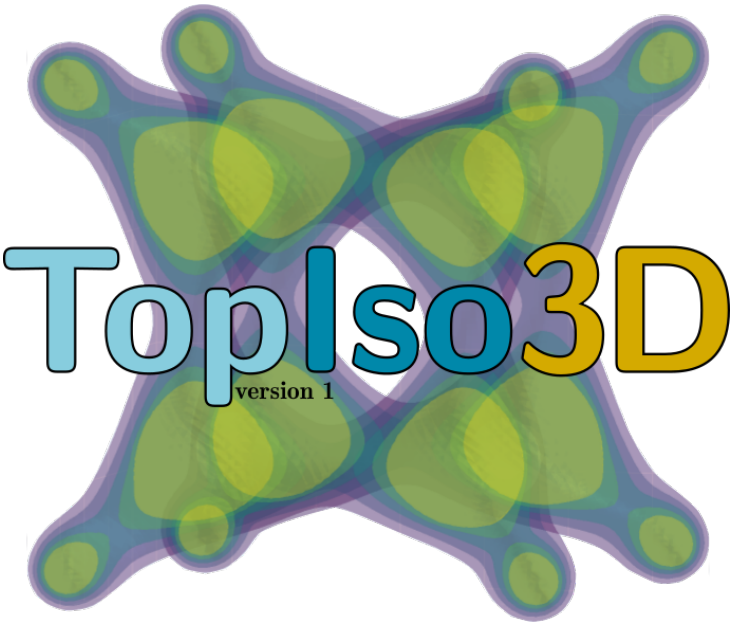
TopIso3D *Viewer v.1*



TopIso3D Viewer User's Manual

[May 21, 2022]

Maia, A. S.[1*], Albuquerque, A. R.[2], Silva J. F.[1]

1 – Chemistry Department, Federal University of Paraíba, PB, Brazil

2 – Chemistry Institut, Federal University of Rio Grande do Norte, RN, Brazil

∗ *Contact author,* arymaia@quimica.ufpb.br

TABLE OF CONTENTS

1 OVERVIEW

TopIso3D *Viewer* was developed in `Python 3.9`, using the modules `Numpy`, `Pandas`, `pdfkit`, `glob`, `os`, `shutil`, `subprocess`, `sys`, `tkinter` and the open source graphics library `Plotly Python` (INC., 2015), in order to allow visualization in 3 dimensions (3D) of the results of topological analysis calculations of molecules and crystalline structures, applying the QTAIM theory (Quantum Theory of Atoms in Molecules) (BADER; ESSéN, 1984), using the Topond software (GATTI; CASASSA, 2014), from the Crystal-17 package (DOVESI et al., 2018).

TopIso3D *Viewer* is based on the automated creation of a sequence of 2D maps, through the PL2D module of TOPOND (GATTI; CASASSA, 2014) and subsequent creation of four-dimensional dataframes, used in the rendering of 3D maps, depending on the user's choices. In addition, TopIso3D *Viewer* has an automation step for launching Topond calculations, in order to create its own data storage structure. The isovalues of the different plotted surfaces, in each 3D map, are not written directly on the image, to avoid a large amount of information, which would make it difficult to understand the structure. In this way, TopIso3D *Viewer* uses a continuous color bar to identify the approximate values of each isosurface.

Version 1 of TopIso3D *Viewer* was developed exclusively to operate in a Linux environment, preferably Ubuntu 18.04. It is made up of three graphical user interfaces (GUI), the Initial GUI, the PL2D GUI and the TopIso3D GUI, which will be further detailed in the next section.

The required citation for this work is:

- **TopIso3D Viewer: Enhancing Topological Analysis through 3D Isosurfaces** Jeronimo F. Silva, Guilherme S. L. Fabris, Julio R. Sambrano, Anderson R. Albuquerque, and Ary S. Maia Journal of Chemical Information and Modeling Article ASAP DOI: 10.1021/acs.jcim.3c00302
- Maia, A.S., Albuquerque, A.R., Silva, J.F.; **TopIso3D Viewer User's Manual**, UFPB, João Pessoa, PB, Brazil, 2022.

2 INSTALLATION AND PREPARATION FOR USE

After downloading the folder with the executable file on your computer, run it inside this folder. There will be all the files necessary for the correct execution of the program.

To use TopIso3D *Viewer* in the visualization of isosurfaces generated by the Topond software (GATTI; CASASSA, 2014) it is necessary that the files generated by this software are available in a particular directory structure and with specific file names. If the user does not have this directory and file structure, TopIso3D *Viewer* has an automation module for launching Topond PL2D calculations (GATTI; CASASSA, 2014), in order to create the directory and file structure necessary for its execution.

Figure 1 exemplifies the structure of directories and files needed to use TopIso3D *Viewer*.

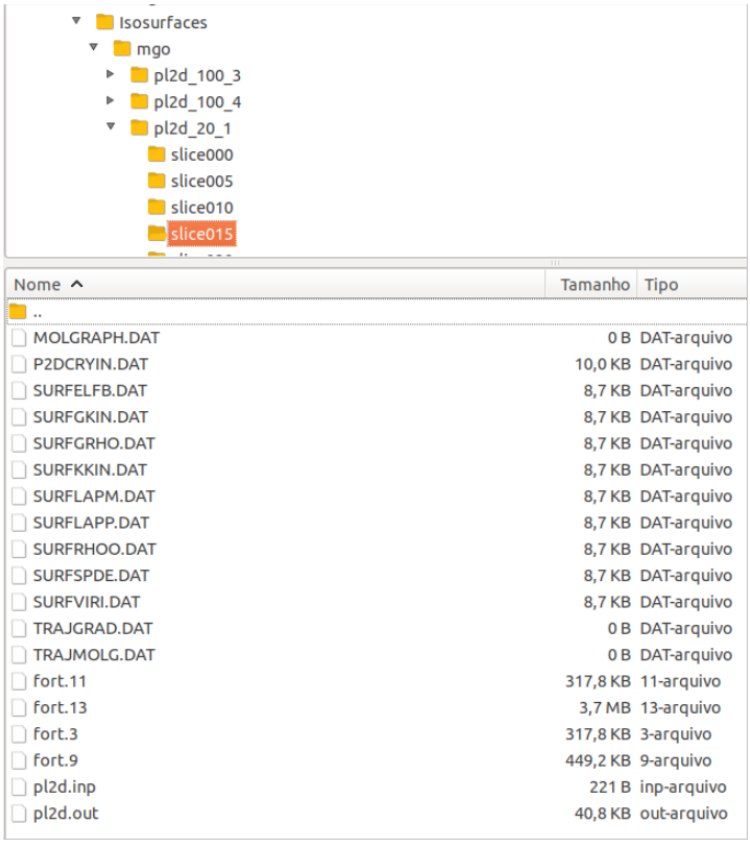


Figura 1 – Necessary structure of folders, to use TopIso3D Viewer.

Whenever the user wants to start the evaluation of isosurfaces of a new structure, he must create a new folder and place the optimized structure's `fort.9` file, generated by the Crystal-17 package (DOVESI et al., 2018) there. Note: If your optimization has generated the file `fort.9`, with another name like `xxxxx.9`, change it to `fort.9`, when placed in the folder. If the user enters the calculation with a name other than `fort.9`, this

will cause an error and a trho folder will be generated. Delete it before starting another attempt. In the example in Figure 1 this folder was `~/Isosurfaces/mgo`. Within it, all the necessary structures for its evaluation will be created.

It is suggested that the evaluation of the data necessary for the automation process be done before starting to use TopIso3D *Viewer*. All the information necessary for the Topond (GATTI; CASASSA, 2014) PL2D calculation will be extracted from the `fort.9` file, opened by the XCrySDen (KOKALJ, 2003) software, for the primitive structure.

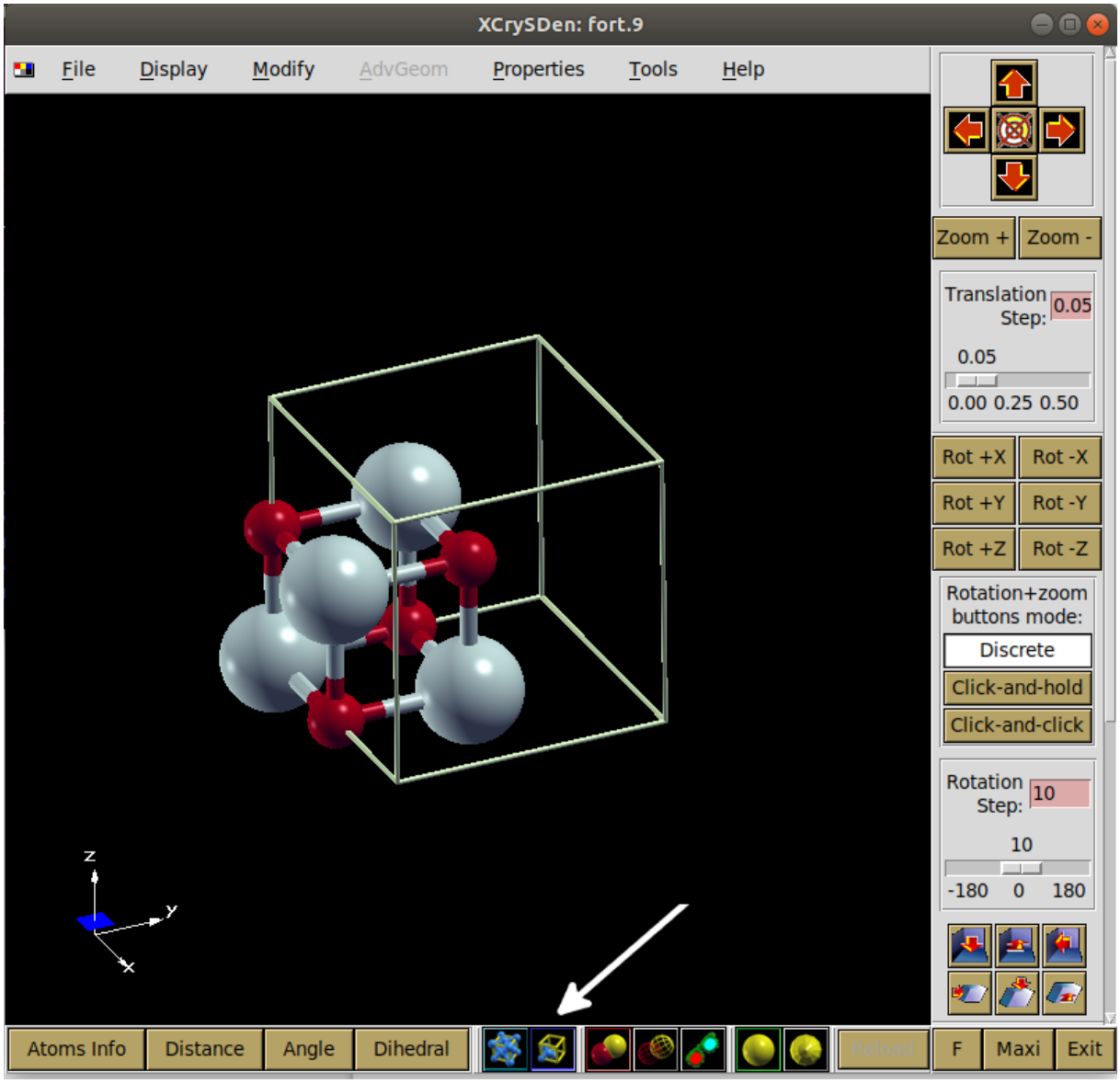


Figura 2 – Example of the MgO primitive structure opened in the XCrySDen (KOKALJ, 2003) software.

Figure 3 exemplifies how to get the necessary data, from the Atoms Info button in the XCrySDen (KOKALJ, 2003), to the MgO structure, taken as an example.

Four atoms were selected, identified by XCrySDen (KOKALJ, 2003), as 1 (Mg), 8 (O), 7 (O) and 4 (Mg), depending on their position in the primitive cell. Atom 1 (Mg) is

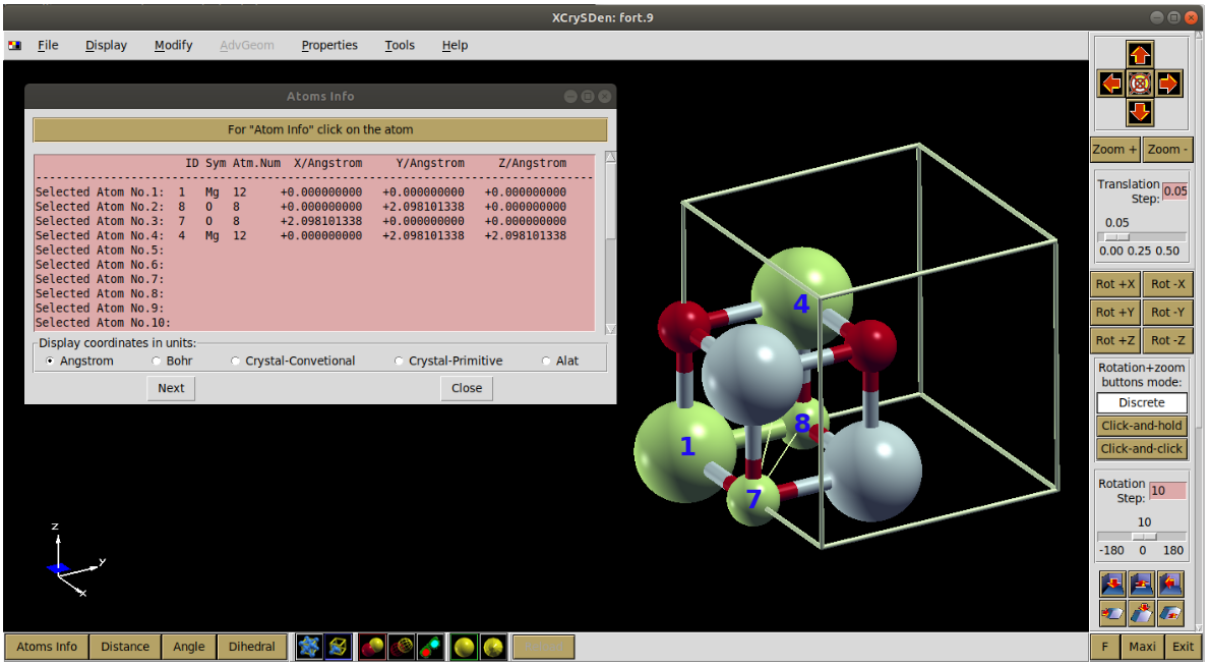


Figura 3 – Obtaining the atomic information for the MgO, through the XCrySDeN (KOKALJ, 2003) software.

the origin of the structure. Atom 7 (O) represents the largest displacement, within the primitive cell, in relation to the x axis. Atom 8 (O) has the same correspondence on the y-axis, while atom 4 (Mg) represents the largest z-value in this cell. The coordinates in Angstroms (Å) are shown in the inset window of Figure 3 .

3 GRAPHICAL USER INTERFACES - GUI:

3.1 Initial GUI

Every time TopIso3D *Viewer* is executed, the first GUI to be opened will ask the user about the existence or not of this directory structure and files, as shown in Figure 4.

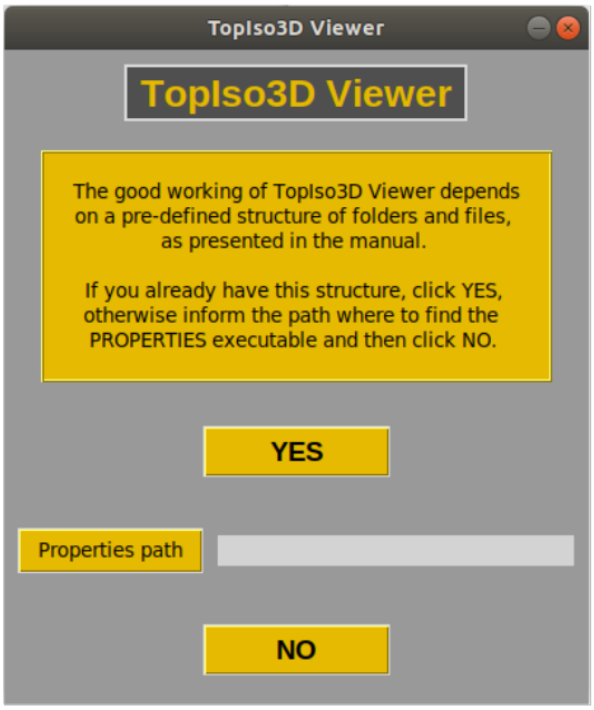


Figura 4 – Initial GUI of TopIso3D *Viewer* software.

If the user already has the necessary data structure, he must click YES. This window will be closed and a new GUI will be opened to inform the data of the isosurfaces to be visualized (TopIso3D GUI). Otherwise, the user must click on Properties path and a window will open for him to look for the path of the executable of the Properties module of the Crystal-17 package (DOVESI et al., 2018), as exemplified in Figure 5.

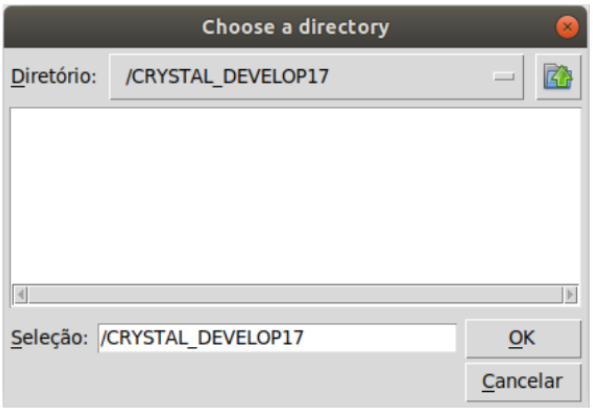


Figura 5 – Window for selecting the properties executable path.

After selecting the path, this address will be written in the Home GUI window and the user must click NO, as exemplified in Figure 6.

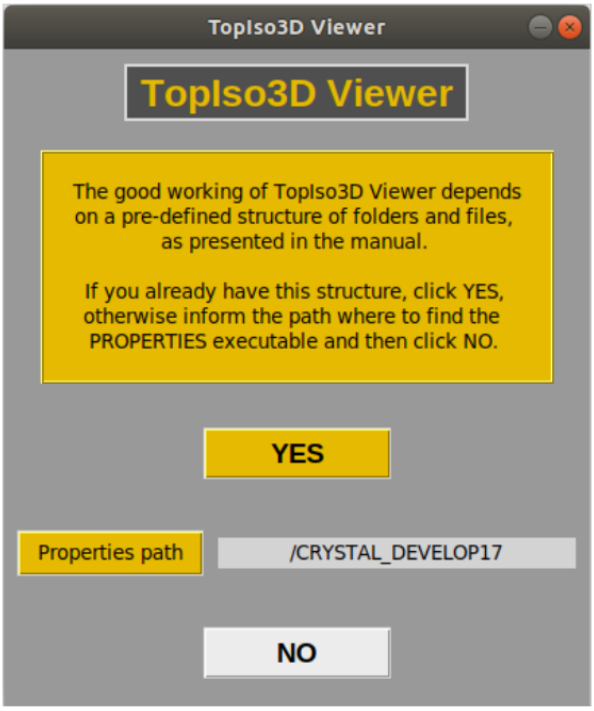


Figura 6 – After selecting the path of the properties executable, click NO, to proceed to the automation of the PL2D calculations.

This GUI will close and a new window will open for automating the launch of the various PL2D calculations, according to the number of slices desired by the user. In this step, the coordinates previously obtained, through the use of XCrySDeN (KOKALJ, 2003) software, would be used.

3.2 PL2D GUI

Users who are familiar with the Topond (GATTI; CASASSA, 2014) software know that the PL2D module's calculations are based on the definition of a plane, starting from three points chosen by the user. The coordinates of these points A, B and C must be informed in the calculation input in order to define the plane in which the isolines of the analyzed property will be created. This is even a sensitive point that makes some visualizations difficult, since the user needs to precisely define the plan to be studied.

As TopIso3D Viewer proposes to create a three-dimensional map of the different topological properties of the structure, from two-dimensional maps calculated by the PL2D module of Topond (GATTI; CASASSA, 2014), this difficulty no longer exists. TopIso3D Viewer will create a series of two-dimensional maps from different xy planes, making the slices grow on the z axis. In this way, points A, B and C can have pre-set coordinates and do not need to be informed by the user.

For information purposes, the coordinates of these three points, used in the TopIso3D Viewer program are A (x=0, y=0), B (x=1, y=0) and C (x=0, y=1), defining different slices as a function of the variations defined in z by the user.

The fact that the final visualization maps of the topological properties are three-dimensional and can be rotated by the user, guarantees the observation of any detail, regardless of the two-dimensional plane in which it had to be calculated by TOPOND (GATTI; CASASSA, 2014).

The automation process for launching the TOPOND calculations includes the PL2D and TRHO modules, since the latter is fundamental in identifying the critical points of the studied system. The input scripts used by TopIso3D Viewer to launch the PL2D and TRHO calculations can be seen in the appendix of this manual (A.1 - PL2D, A.2 - TRHO).

Figure 7 presents the GUI for automating PL2D calculations, using the TOPOND (GATTI; CASASSA, 2014) of the CRYSTAL package (DOVESI et al., 2018).

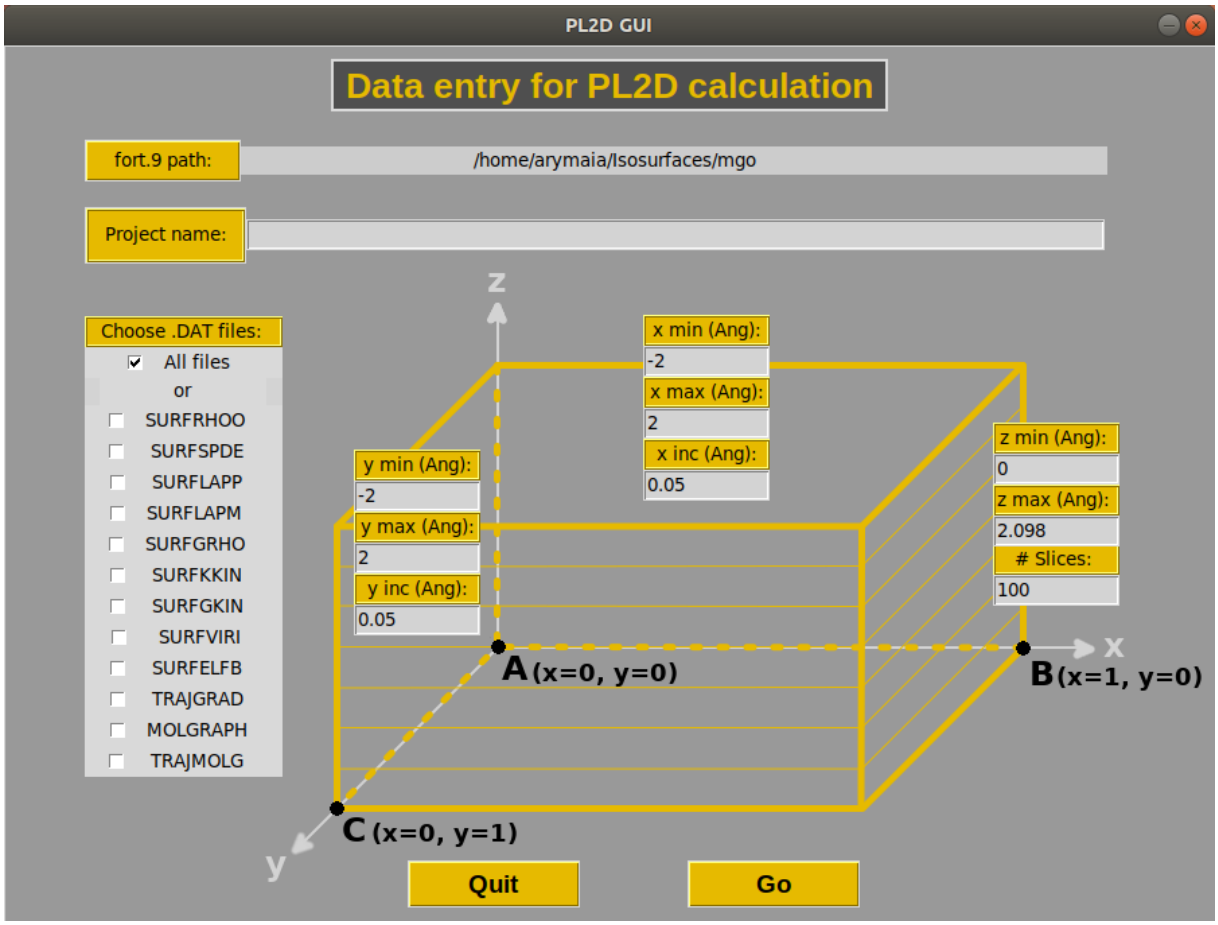


Figura 7 – GUI of the PL2D calculation automation module.

Following the TOPISO3D *Viewer* filling sequence, all the windows of this GUI will be displayed, as follows:

1. fort.9 path : By clicking on this button, a window will open to choose the path of the folder where the optimized structure fort.9 is located, which will be used in the automation process.

2. Choose .DAT file : As with the manual launch of TOPOND's PL2D calculations [3], TopIso3D *Viewer* allows the user to choose which types of scalar functions will be calculated. The user can choose All files , or any combination of the options presented.

3. x min (Ang) e x max (Ang) : The user must indicate the presentation interval of the isosurfaces to be calculated. You can indicate the values used in the definition of points A, B and C, or alternatively, different values, in case the user is interested in observing a specific detail within its structure or even a wider region of the system. In the example, isosurfaces will be plotted in the range -2 Å $<$ x $<$ 2 Å.

4. x inc (Ang) : The user must present the increment that will be applied within the limit of the values of x min and y min, in the calculation of the isosurfaces. Low values imply higher resolution on the axis, but higher computational cost. It is suggested to start the evaluation with values around 0.1.

5. y min (Ang) , y max (Ang) e y inc (Ang) : Similar to x min (Ang) , x max (Ang) and x inc (Ang) windows. Regardless of the type of crystallographic system to which the analyzed structure belongs, it is strongly recommended that the values of these variables for x and y are the same, since TopIso3D *Viewer* uses the formation of a square matrix to create the n slices to be evaluated. This type of choice does not affect the final visualization of whatever the crystallographic system of the structure.

6. z min (Ang) and z max (Ang) : In this field, the user must inform the z coordinate interval, where the program will create the number of slices selected in # Slices . In the example presented, 100 slices would be created between z = 0 Å and z = 2,098 Å. TopIso3D *Viewer* will use this value and the number of slices to calculate the z coordinates for the selected n slices.

7. # Slices : In this window, the user will indicate the number of slices that will be used in the n PL2D calculations of Topond (GATTI; CASASSA, 2014). TopIso3D *Viewer* is programmed to accept 20, 50 or 100 slices, depending on the desired z-axis resolution. The use of 20 slices is recommended for very heavy structures, or when a first evaluation of three-dimensional isosurfaces is desired. The use of 100 slices guarantees good resolution on the z axis.

Before proceeding with the calculations, it is advisable for the user to make sure that the various PL2D calculations in Topond (GATTI; CASASSA, 2014) have already been

completed. The duration of this step will vary with the complexity of the structure and the degree of accuracy desired (depending on the values defined in relation to x inc (Ang), y inc (Ang) and # Slices. The completion confirmation can occur through the use of from the `top` command, in the linux command line, confirming, in the Table of Processes, that all the properties calculations are finished.

After finishing the calculation with properties, a subfolder is created, in the original folder, which contained the file `fort.9`, where the folders referring to the number of slices created will be. This folder will be named `pl2d_xxx_y`, where the value of `xxx` will indicate the number of slices used and y is an automatic count of these folders. The example used in Figure 7 generated the folder `pl2d_100_17`, which means that inside it there are 101 folders referring to the 100 slices defined previously, in addition to a `trho` folder where the files generated by the **Topological Analysis of the Electron Density (TRHO)** calculation are located, as performed in TOPOND (GATTI; CASASSA, 2014). In each folder named `slicezzz` (where `zzz` indicates the slice number) are the files generated as a result of the **Plotting functions in 2 dimension (PL2D)** calculation, presented previously in Figure 1, as a result of the choice made in Choose .DAT file. Each of these files can be viewed in 2D, without any problem, by CRYSPLOT (on <http://crysplot.crystalsolutions.eu/>). This folder structure can be seen in Figure 8.

3.3 TopIso3D GUI

Finally, a last GUI will be opened, named TOPISO3D *Viewer*, where the data for the generation of the image of the desired isosurfaces will be placed, as shown in Figure 9.

The TOPISO3D *Viewer* GUI requires filling in a series of fields, as described below:

1. Directory: Where the user must select the Path of the `pl2d_xxx_y` folder, where all the calculated slices folders are. In the example used: `~/mgo/pl2d_100_17`.

2. Choose the topological isosurface: The user must choose one of the different types of isosurfaces presented. The choice will be automatically written in the Isosurface selected field. In the example shown, the isosurface was SURFRHOO - Electron density. It is worth remembering that the user must choose the type of isosurface, taking into account whether it was calculated in the PL2D GUI step. Choosing an isosurface type that has not been previously calculated will result in an error.

3. Choose the Number of Slices: The user must choose the number of slices calculated for this directory. The choice will be automatically written in the Number of slices field. In case of doubt, the user can consult the number of slices present in the name of the folder selected in Directory. In the example shown, there were 100 slices.

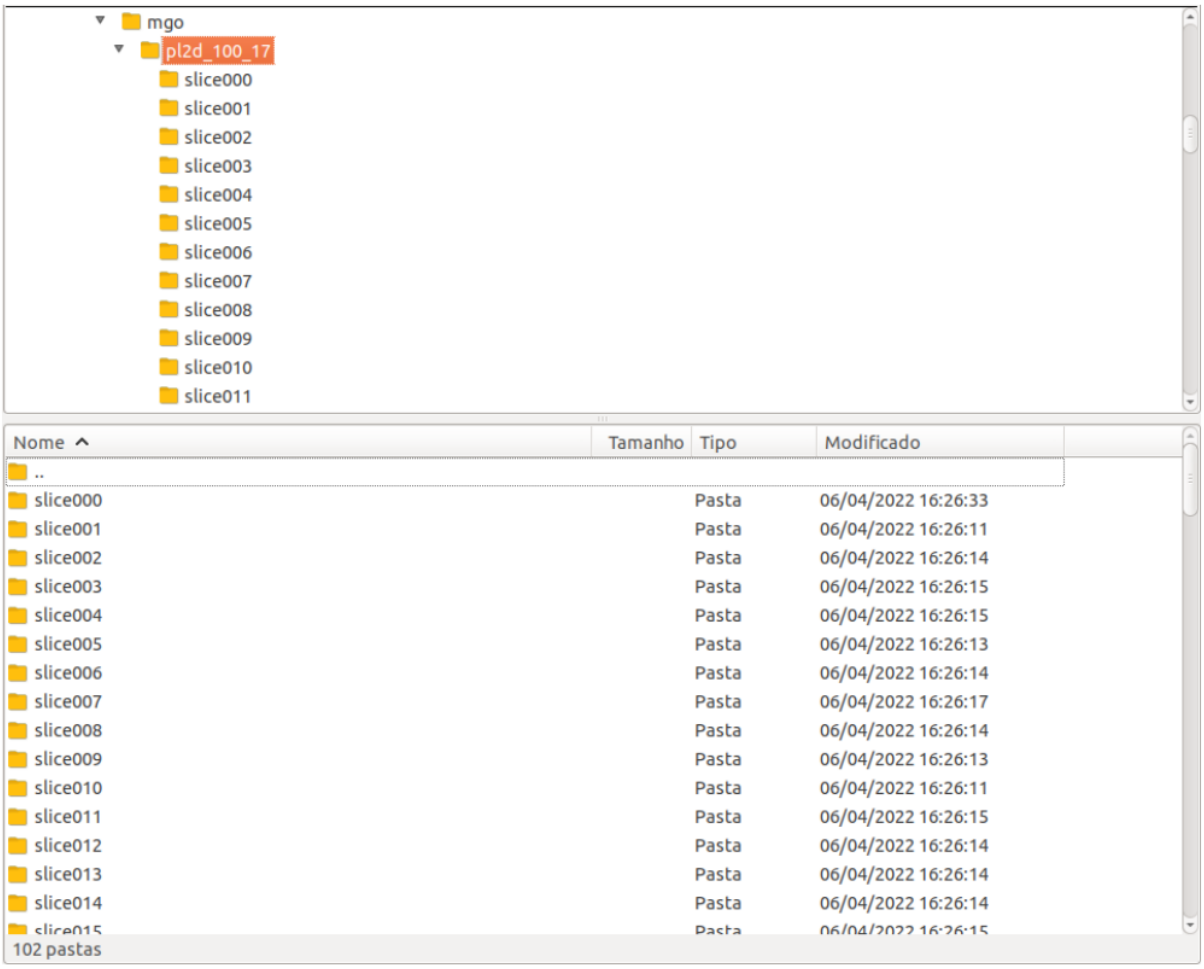


Figura 8 – Folder structure created automatically by the TopIso3D *Viewer* software.

4. Choose the number of isosurfaces: The user must type the number of isosurfaces desired in the rendering of the figure and click on Done. At this moment the value entered will be shown below the button, *e.g.*: Number of isosurf. selected: 3. It is worth remembering that a large number of isosurfaces can make it difficult to understand the image to be generated, as it is a 3D map, in addition to increasing the computational cost of the rendering step.

5. Choose the opacity (0 to 1): The user must enter the opacity of the isosurfaces to be rendered and click on Done. At this moment the value entered will be written in the window below the button. The opacity value must be fractional, as explained in the caption. In the example shown, an Opacity: 0.1 was chosen (10% opacity or 90% transparency).

6. Choose the minimum and maximum topological isosurface: The user must enter the minimum and maximum values for the isosurfaces to be rendered and click on Done. The sentence The isosurfaces will be plotted between `xxx` and `yyy` will be written below the button. In the example shown, the minimum and maximum values

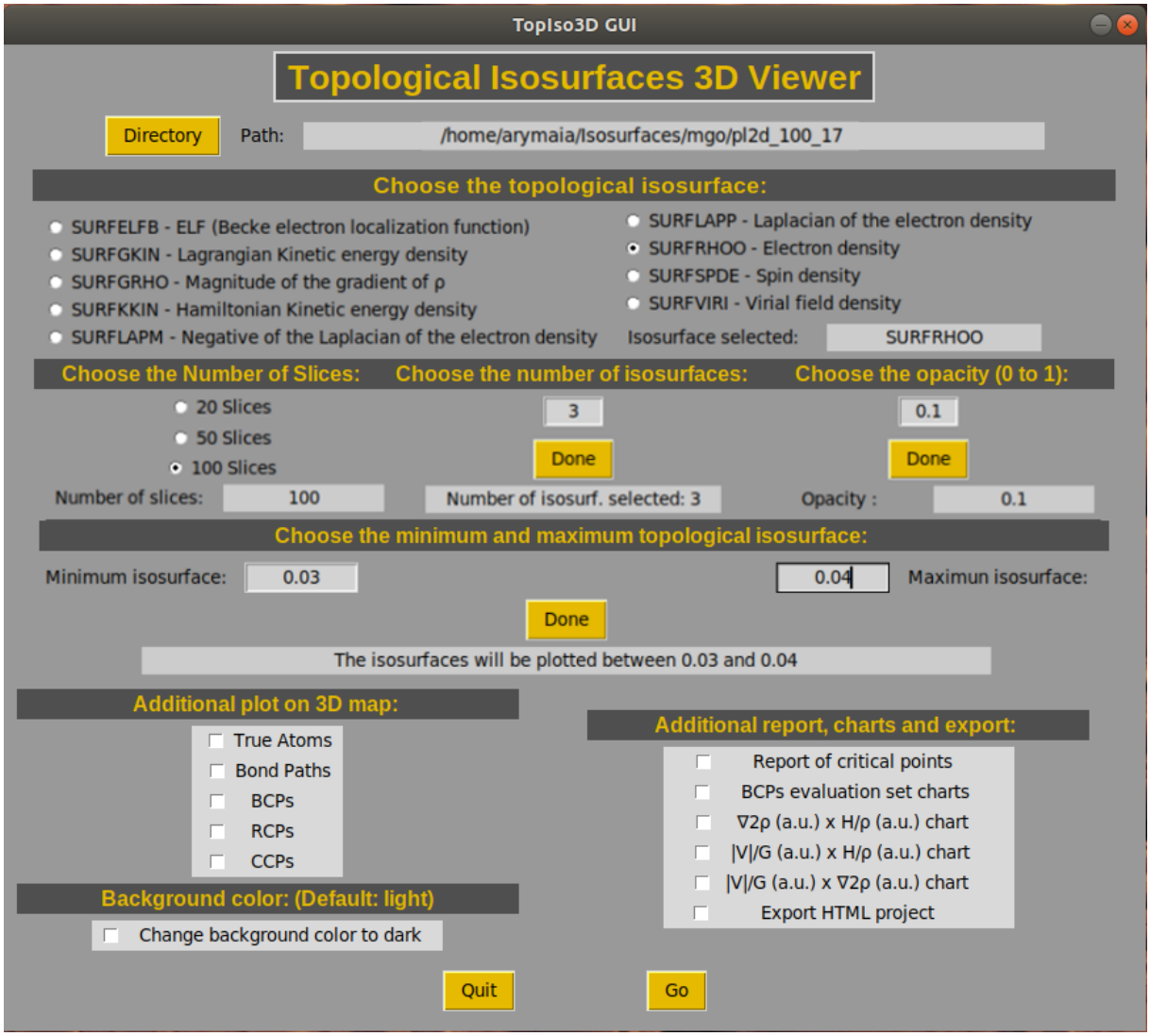


Figura 9 – TopIso3D *Viewer* GUI

were 0.03 and 0.04 (a.u.).

7. Additional plot on 3D map : The user will be able to choose among the types of critical points presented, those that he wants to be plotted along with the isosurfaces. They are:

   - True Atoms : only the True atoms of the structure will be plotted
   - NNAs : Non-nuclear attractors
   - BCPs : Critical connection points
   - RCPs : Ring Critical Points
   - CCPs : Cage Critical Points

   This functionality is well adapted for the case where the plot limits, represented by the values x, y and z (min and max), are coincident with the cell parameters. In situations where the plot limits and the unit cell are not coincident or for some

structures a little more complex, an error may occur when plotting these critical points. If this occurs, it is suggested that no Additional plot option is selected. Appendix A.3 presents a figure referring to the structure studied as example (MgO), highlighting the plotting of its critical points.

8. Background color: (Default: light) : The background color can be changed from light (default) to dark. This feature is useful when the set of isosurfaces to be plotted has one that falls in a very light region in the color scale.

9. Additional report, charts and export : The user will be able to choose from the following options:

   - Report of critical points : The user will generate a Synthetic report of all critical points, with their coordinates and an evaluation of the BCPs regarding their character. This report will be saved in the `pl2d_xxx_y` folder, with the name `final_report.xlsx`. As the **Critical Points Information** is taken from the **Topological Analysis of the Electron Density (TRHO)** calculation and is independent of the isosurface calculation, once it has been generated, it does not need to be repeated, unless a new calculation is performed at a later date from a new `fort.9` file.
   - BCPs evaluation set charts : Three graphs will be generated where the BCPs will be plotted according to the descriptors $\nabla^2\rho$, $|V|/G$ and H/ρ (GATTI; SAUNDERS; ROETTI, 1994), two by two, in order to help classify the type of chemical interaction represented by the respective BCP.
   - $\nabla^2\rho_b$ (a.u.) x H/ρ_b (a.u.) chart : All BCPs of the analyzed structure will be plotted on a $\nabla^2\rho_b$ x H/ρ_b graph and a statistical dispersion analysis will be made of these points on both axes.
   - $|V_b|/G_b$ (a.u.) x H/ρ_b (a.u.) chart : All BCPs of the analyzed structure will be plotted on a $|V_b|/G_b$ x H/ρ_b graph and a statistical dispersion analysis will be made of these points on both axes.
   - $|V_b|/G_b$ (a.u.) x $\nabla^2\rho_b$: All BCPs of the analyzed structure will be plotted on a $|V_b|/G_b$ x $\nabla^2\rho_b$ graph and a statistical dispersion analysis will be made of these points on both axes.
   - Export HTML project : This option allows the 3D map project to be saved in the form of an HTML file, in the source pl2d_xxx_y folder, allowing the user to open it later, through any browser, for a new visualization/evaluation.

After filling all the fields, the user must click on the Go button and TopIso3D *Viewer* will start the process of rendering the 3D map of the isosurfaces, using the default

browser of the user's computer. It is recommended to use the *Firefox* browser, as it proved to be faster in rendering/manipulating images.

The map generated with the three-dimensional isosurfaces is intuitive to use and is rich in detail. Precisely for this reason, it is necessary to carefully choose the defined parameters, both in the PL2D calculation automation stage (PL2D GUI), and in the 3D isosurface map generation stage (TopIso3D GUI), in particular with regard to the number of isosurfaces to be plotted, the maximum and minimum limits of the isosurfaces and the opacity. Figure 10 shows some views of the 3D map created from the example.

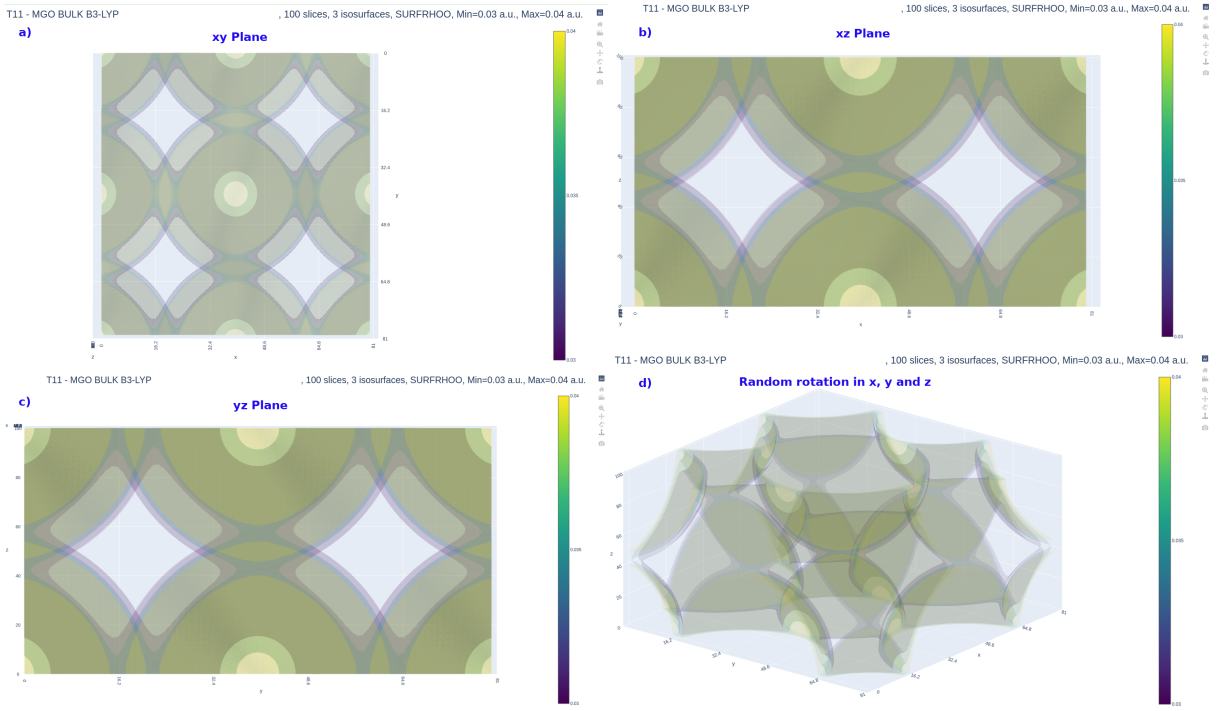


Figura 10 – Different views of the 3D isosurface map generated by TopIso3D *Viewer*. a) xy plane, b) xz plane, c) yz plane and d) view with a random rotation in x, y and z.

TopIso3D *Viewer* generates a 3D map that can be rotated in any of the axes, by moving the mouse, with the left button pressed, and can be enlarged or reduced with the help of the mouse scroll. Each generated 3D map occupies a new browser tab.

In each map, it is possible to identify a header with information such as the title of the studied system, as presented in the fort.9 file of the optimized structure, the number of slices, the number of isosurfaces, the type of isosurface chosen, with the nomenclature used by the Topond (GATTI; CASASSA, 2014) and the maximum and minimum limits used in rendering the image. These limits, maximum and minimum, are also shown in the continuous color bar, on the right of the map.

In the upper right corner, the `Plotly` (INC., 2015) modebar can be seen, which allows a series of manipulations of the 3D map created, through the set of icons shown in

Figure 11. The map can be manipulated, through processes of orbital rotation, rotation about an axis, translation, zoom, etc., for better visualization and understanding of the evaluated system. For more information about each of the functions presented, see <https://plotly.com/python/>.

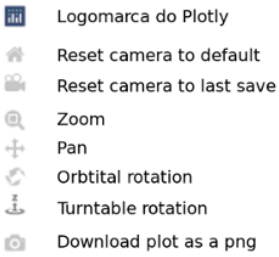


Figura 11 – `Plotly` (INC., 2015) modebar functions, presented in TopIso3D *Viewer*.

Figure 12 presents the BCPs Evaluation graph, generated from the example used and a fragment of the report recorded in the file `final_report.xlsx`, in the form of a spreadsheet, with several individualized sheets:

- primitive : with information about atomic positions in the primitive cell
- true_atoms : with information about atomic positions of the true atoms of the structure
- bcp : with information about atomic positions of the bond critical points
- properties : with the identification of the atoms involved in each BCP and the values of the descriptors employed in the classification of chemical interactions
- nna : with information about atomic positions of the non nuclear attractors
- rcp : with information about atomic positions of the ring critical points
- ccp : with information about atomic positions of the cage critical points

From the trho calculation performed by Topond (GATTI; CASASSA, 2014) two different BCPs were identified for the MgO structure, used as an example, as shown in Figure 12(b). The report identifies the chemical elements involved in these interactions along with presents the values of each descriptor for them (`LAP`, `ADIM_RATIO`, `BOND_DEGREE` and `RHO`). From the graphs presented in Figure 12(a) it is possible to identify the degree of covalence of the interaction, as well as its character between Shared-shell, Closed-shell or Transit region, as proposed by Espinosa and collaborators (ESPINOSA et al., 2002).

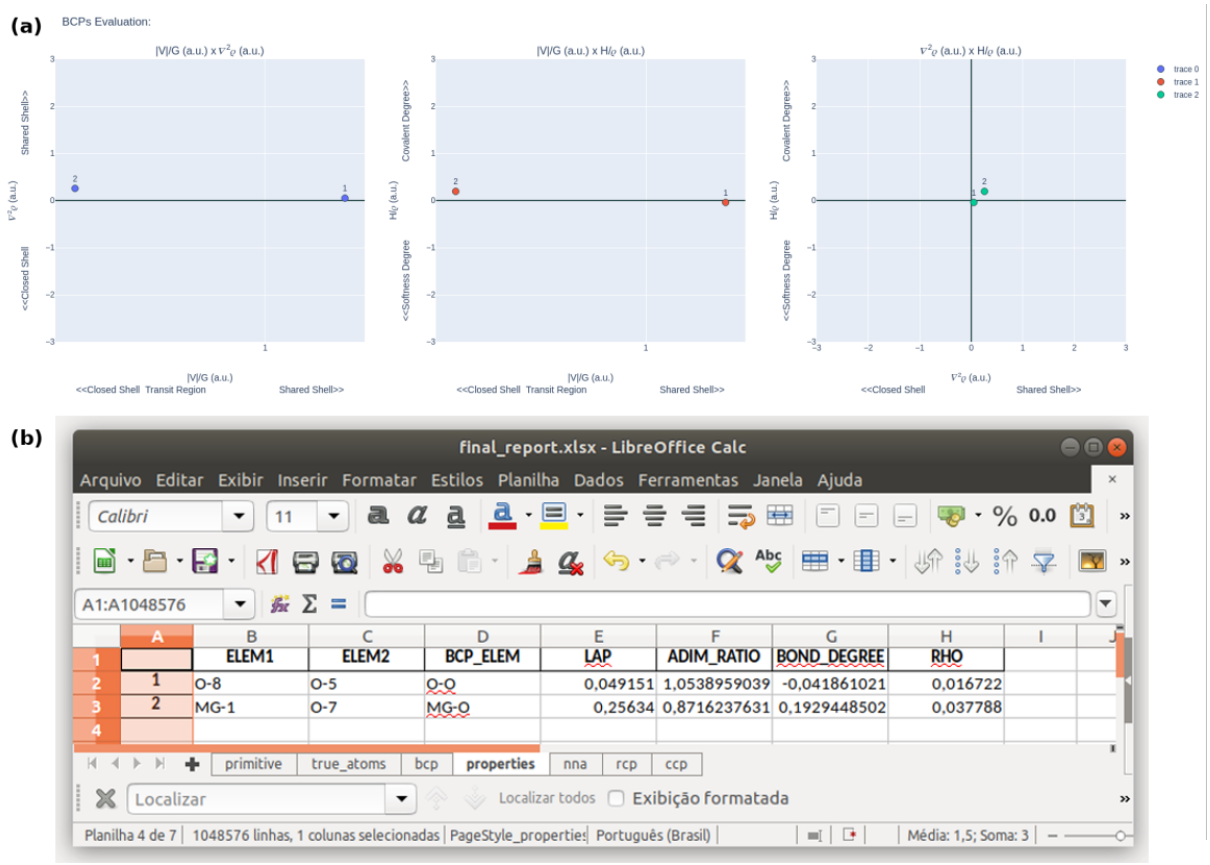


Figura 12 – BCPs evaluation charts of structure (a) and fragment of the Critical Points Report (b).

3.3.1 On choosing the number of isosurfaces

One of the most sensitive parameters for a good understanding of the 3D isosurface map is the number of isosurfaces chosen. Figure 13 presents a series of 3D maps, for the example used previously, working with fixed values of the maximum and minimum limits and varying the number of isosurfaces from 1 to 5.

The first important observation concerns the range of colors in each of the figures. As the minimum and maximum values were maintained (from 0.01 a.u. to 0.1 a.u.) for all maps, different numbers of isosurfaces will imply plotting isosurfaces with different isovalues and consequently different colors, mainly for figures (a), (b) and (c). From this, the amount of isosurfaces already allows the colors to be relatively maintained.

A second important observation is that, for these minimum and maximum limits defined for electron density isosurfaces, a smaller number of isosurfaces did not lead to the observation of the interaction between Mg and O atoms.

On the other hand, as in Figure 13(e), it is clearly observed that this interaction occurs around an electron density of 0.03 a.u., one can think of generating a 3D map with a single isosurface, working with the minimum and maximum equal, in order to evidence

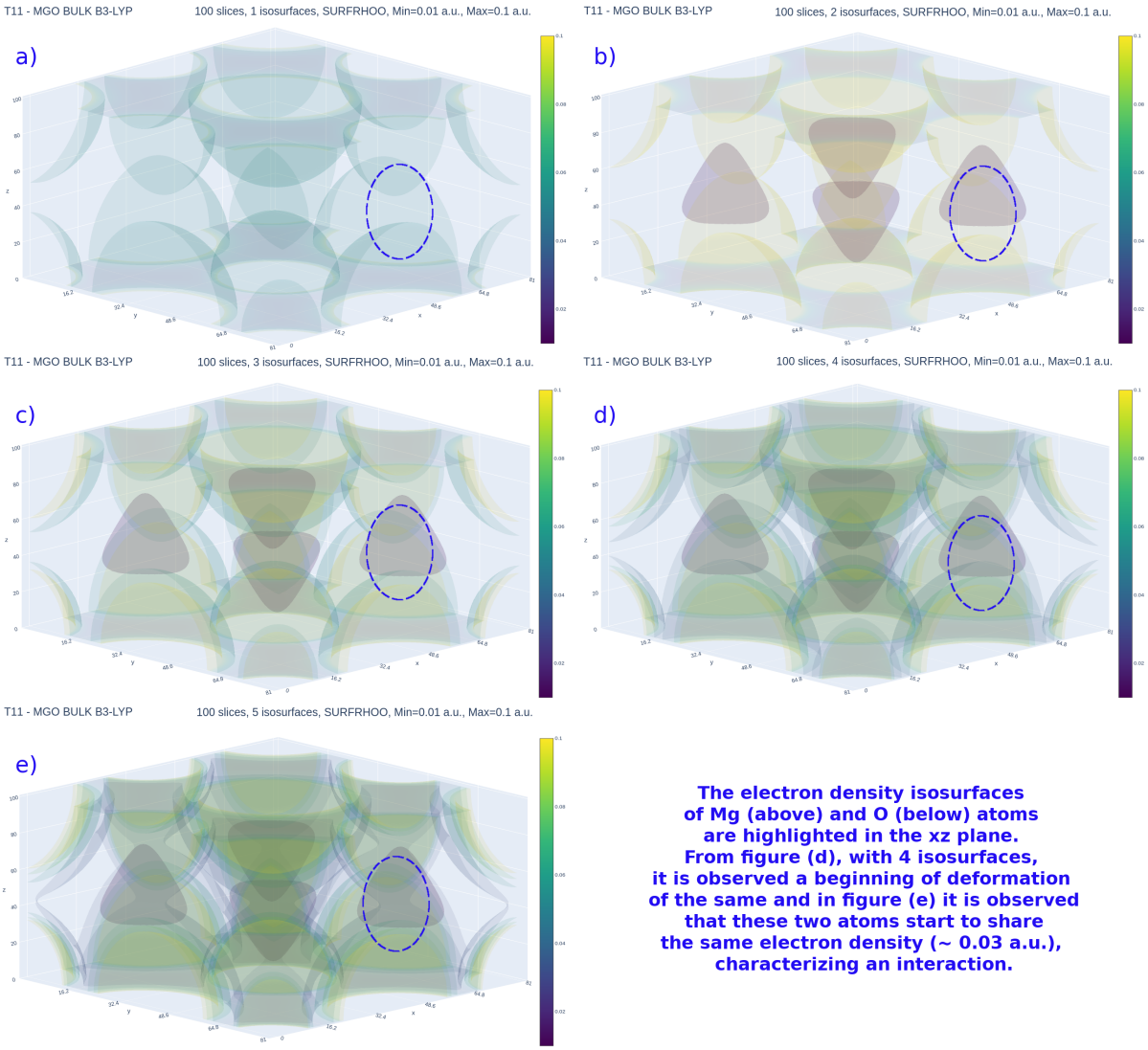


Figura 13 – Evaluation of the influence of the number of isosurfaces on the plotting of maps.

this interaction, as in Figure 14. The exact value of electronic density referring to this BCP (0.03779 a.u.) can be seen in Figure 12(b), as part of the Critical Points Report.

This figure highlights the interactions between several Mg and O atoms, distributed in the intermediate region of the cell chosen for plotting. It is observed that this isosurface is common to all atoms of this cell, indicating that the interaction between them presents the same electron density. It is worth noting that, when viewed at certain angles, as in Figure 14.a which shows the xy plane, these interactions behave like holes in the electronic isodensity envelope, characterizing that this isosurface is common to atoms located in the upper fraction and bottom of this cell.

This procedure of working with a single surface can even be used to plot the electron density isosurface in the value of a BCP of the structure, as shown in Figure 15, where the red highlights indicate the position of the BCP.

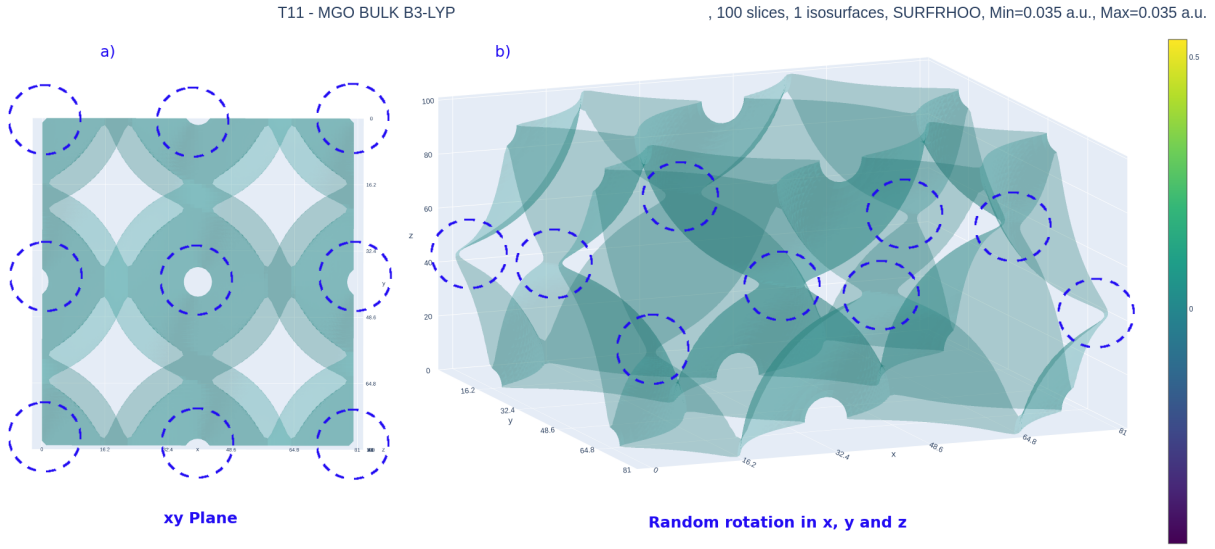


Figura 14 – Single isosurface of electron density equal to 0.035 a.u. for MgO.

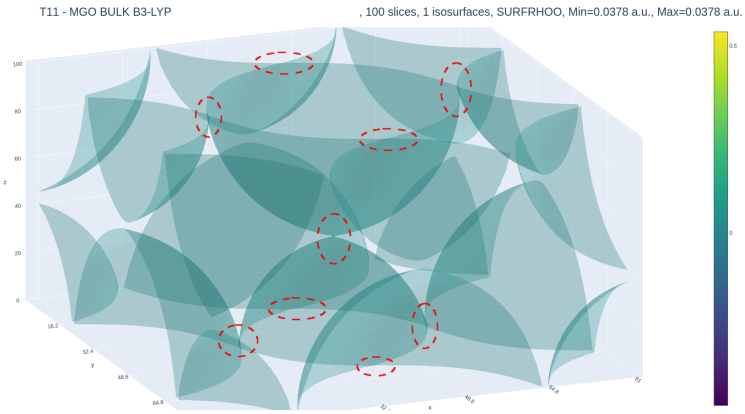


Figura 15 – Visualization of the BCP on the isosurface with electron density equal to 0.0378 a.u. for MgO.

3.3.2 On choosing the minimum and maximum limits of isosurfaces

Another extremely important parameter in defining the image is the minimum and maximum values of the isosurface used in the generation of the 3D map. Figure 16 uses the same previous example, setting the number of isosurfaces to 3 (three), but working with different electron density intervals. The different minimum and maximum limits used in each of the five figures were (a) Min = 0.001 a.u. and Max = 0.3 a.u.; (b) Min = 0.001 a.u. and Max = 0.1 a.u.; (c) Min = 0.001 a.u. and Max = 0.01 a.u.; (d) Min = 0.01 a.u. and Max = 0.1 a.u.; (e) Min = 0.01 a.u. and Max = 0.05 a.u..

This result highlights the need to carefully adjust the values of the isosurface limits, in order to allow highlighting the detail that is desired to be visualized.

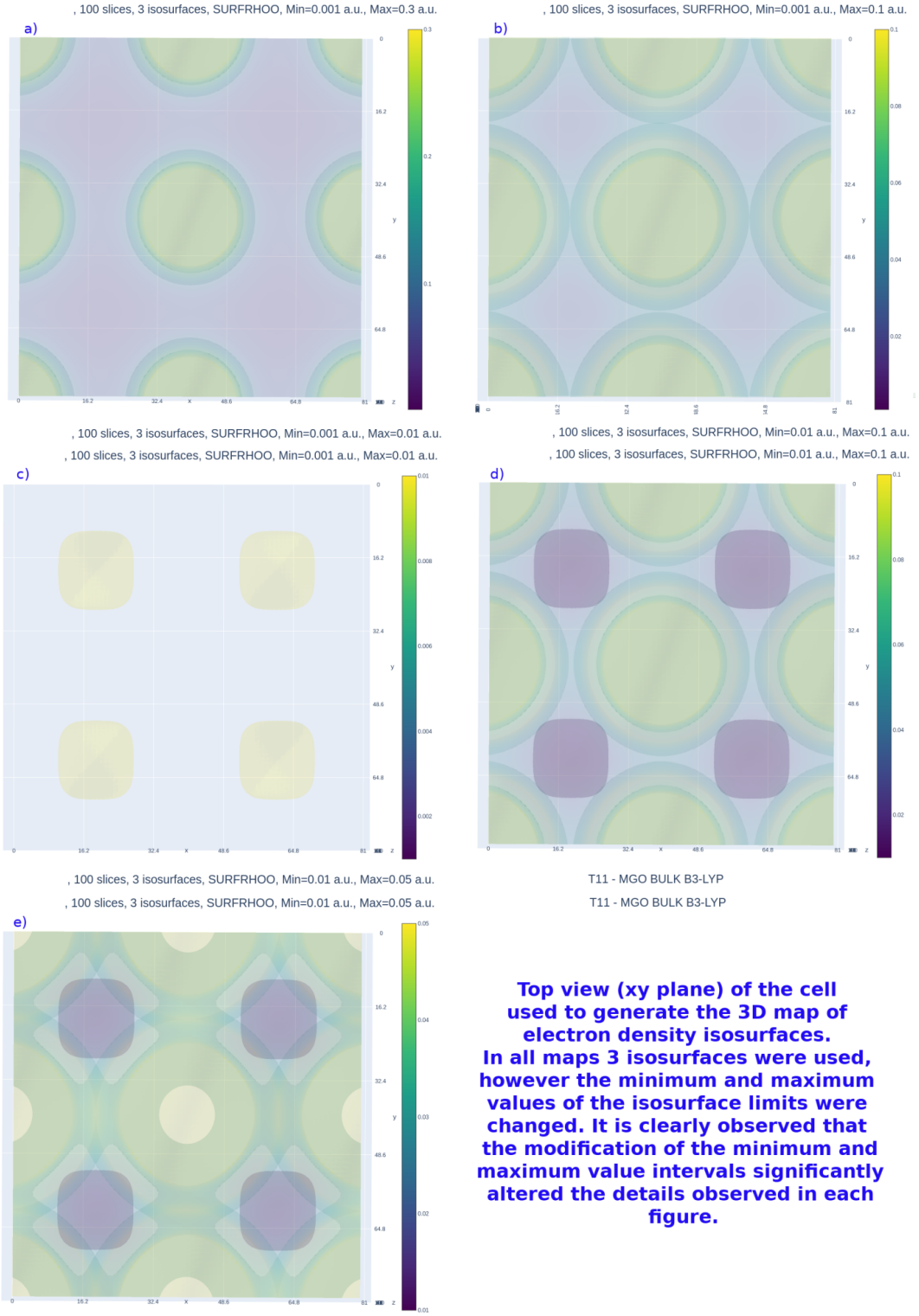


Figura 16 – Evaluation of the influence of the minimum and maximum limits of isosurfaces on the plotting of 3D maps.

REFERENCES

BADER, R. F. W.; ESSéN, H. The characterization of atomic interactions. *The Journal of Chemical Physics*, v. 80, n. 5, p. 1943–1960, 1984. Disponível em: <https://doi.org/10.1063/1.446956>.

DOVESI, R. et al. Quantum-mechanical condensed matter simulations with crystal. *WIREs Computational Molecular Science*, v. 8, n. 4, p. e1360, 2018. Disponível em: <https://wires.onlinelibrary.wiley.com/doi/abs/10.1002/wcms.1360>.

ESPINOSA, E. et al. From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving x–hf–y systems. *The Journal of Chemical Physics*, v. 117, n. 12, p. 5529–5542, 2002. Disponível em: <https://doi.org/10.1063/1.1501133>.

GATTI, C.; CASASSA, S. *TOPOND User's Manual*. Milano: CNR-ISTM of Milano, 2014.

GATTI, C.; SAUNDERS, V. R.; ROETTI, C. Crystal field effects on the topological properties of the electron density in molecular crystals: The case of urea. *The Journal of Chemical Physics*, v. 101, n. 12, p. 10686–10696, 1994. Disponível em: <https://doi.org/10.1063/1.467882>.

INC., P. T. *Collaborative data science*. Montreal, QC: Plotly Technologies Inc., 2015. Disponível em: <https://plot.ly>.

KOKALJ, A. Computer graphics and graphical user interfaces as tools in simulations of matter at the atomic scale. *Computational Materials Science*, v. 28, n. 2, p. 155–168, 2003. ISSN 0927-0256. Proceedings of the Symposium on Software Development for Process and Materials Design. Disponível em: <https://www.sciencedirect.com/science/article/pii/S0927025603001046>.

A APPENDIX

A.1 Input for the PL2D calculation of slice000:

```
TOPO
PL2D
0
0.0 0.0 0.0
0
1.8897261339212517 0.0 0.0
0
0.0 1.8897261339212517 0.0
3
0
30, 15.0
1
-2.0 2.0 0.05
-2.0 2.0 0.05
1,1,1,1,1,1,1,1,1,1,1,1
mgo
1
2.0,0.0, 0
2.2,1,1,1
36,0
END
```

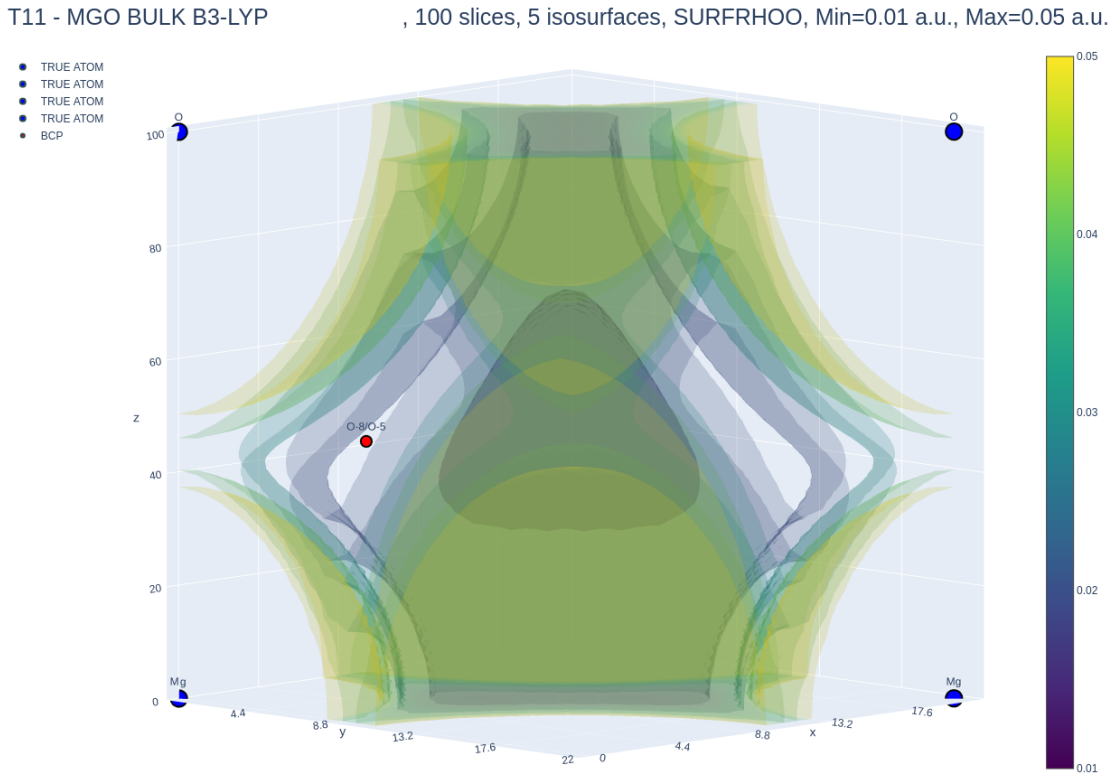
A.2 Input of TRHO calculation:

```
TOPO
TRHO
-1
1,0,1,0,20,10,10.,5.
END
```

A.3 Additional plot:

Figure 17 exemplifies the additional plot of True Atoms and BCPs for the structure used as an example in this manual (MgO). It also presents fragments of *final_report.xlsx*, regarding these critical points calculated by TOPOND (GATTI; CASASSA, 2014).

It is important to note that, for the critical points to be plotted correctly, it was necessary to modify the plot parameters (x, y and z min and max) in order to represent the primitive cell of the structure, when launching the PL2D calculations (Figure 7).



True Atoms Sheet:

	A	B	C	D	E	F	G	H	I	J
1		ELEMENT	x_ANGSTROM	y_ANGSTROM	z_ANGSTROM	pt_atom_x	pt_atom_y	pt_atom_z		
2	1	12	0	0	0	0	0	0		
3	2	12	2,098187631	2,098187631	0	21	21	0		
4	3	8	0	0	2,098187631	0	0	100		
5	4	8	2,098187631	2,098187631	2,098187631	21	21	100		

primitive | true_atoms | bcp | properties | nna | rcp | ccp

BCPs Sheet:

	A	B	C	D	E	F	G	H	I	J
1		x_ANGSTROM	y_ANGSTROM	z_ANGSTROM	pt_bcp_x	pt_bcp_y	pt_bcp_z			
2	1	0	1,049	1,049	0	10	50			
3	2	-3,3	0	0	-33	0	0			

primitive | true_atoms | bcp | properties | nna | rcp | ccp

Figura 17 – Additional plot of True Atoms and BCPs stops in the primitive cell of the MgO associated with the tables with their coordinates.

The figure was randomly rationed in order to allow the visualization of the four True Atoms at the vertices of the structure. Even taking care to use the parameters of the primitive cell, it is observed that the BCP number 2 was calculated by TOPOND (GATTI; CASASSA, 2014), outside the limits of this structure, not being plotted in this figure.