

MedeA: Structure List Editor: Manage Your Structure Repository With Properties

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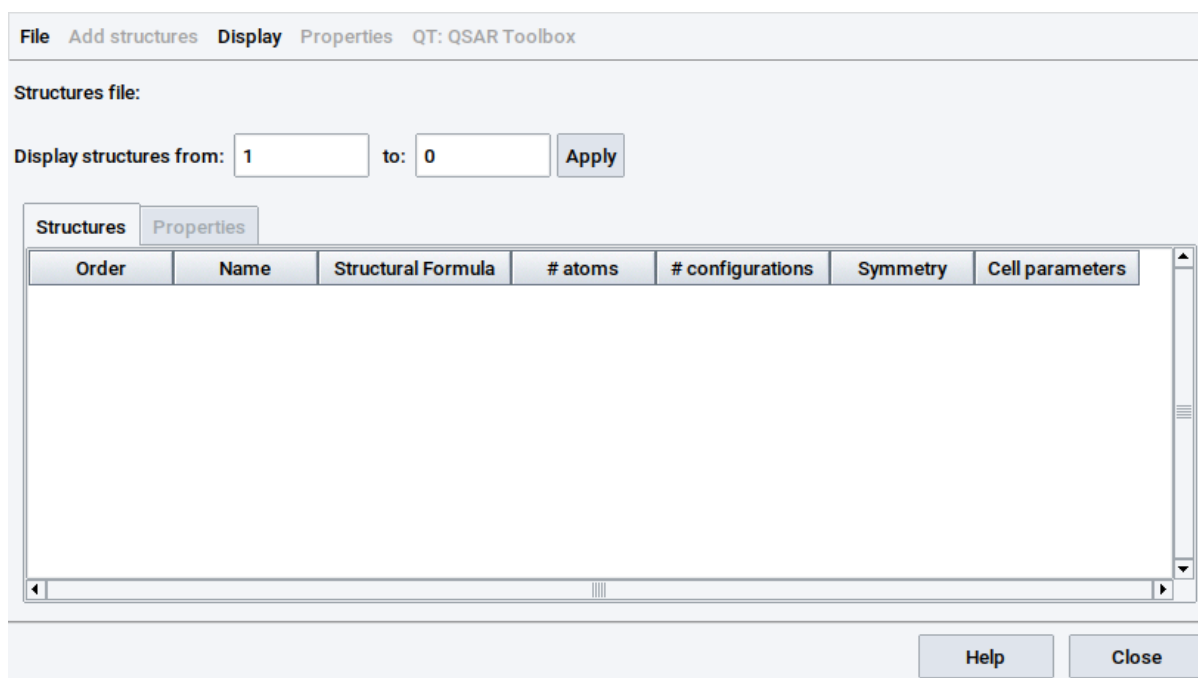
1 Introduction

Define a list of structures, with arbitrary configurations, compositions and associated properties and descriptors. Structures can be simple molecules, a fluid (ensemble of molecules to form a gaseous or liquid state), or solids in a crystalline or an amorphous state. Structure lists are stored as a single file either in the database format SQLite or as clearly readable text in the ASCII format. With structure list you can archive and store your calculated results (properties, descriptors) together with structures that are used to calculate the properties. Also use structure lists to leverage the power of flowcharts to perform high-throughput (HT) screening and use HT applications). For HT calculations, use the *MedeA* module *HT-Launchpad* and the flowchart stage **Foreach Structure Loop** to apply the same compute workflow on each record of the structure list. With this you can obtain consistently calculated data. Another application of structure lists is to predict properties of compounds using correlations with the *MedeA* modules *HT-Descriptor* and *QT*. The latter is the *MedeA* QSPR Toolbox, that employs an interactive graphical user interface to allow you to explore and analyze the relationships between descriptors, structural properties, and materials properties.

For more information about structure lists in the context of high-throughput calculations read the Section MedeA HT.

In case you are interested to use structure lists in conjunction with *MedeA QT* then read Section MedeA QT.

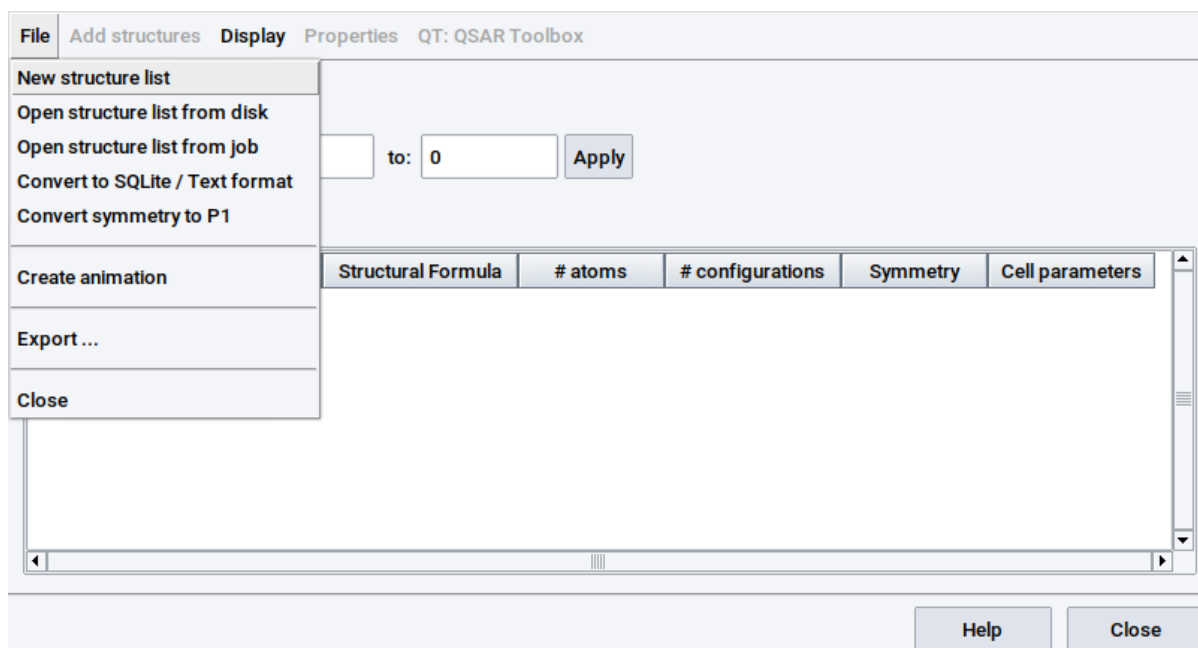
The structure list editor is opened in the *MedeA GUI* with **File >> Structure List Editor**. Without any structure list loaded the invoked dialogue looks such as depicted in the below image.



Note: Every structure list editor can handle only one structure list. However, you can open several structure list editors in parallel via **File** >> **Structure List Editor**.

2 Handle Entire Structure Lists

An entire structure list can be handled via **File** menu item of the structure list editor. You can create a new and empty structure list, open existing structure lists, convert structure lists and their entire content, and export the properties of the structure list to a file on disk:

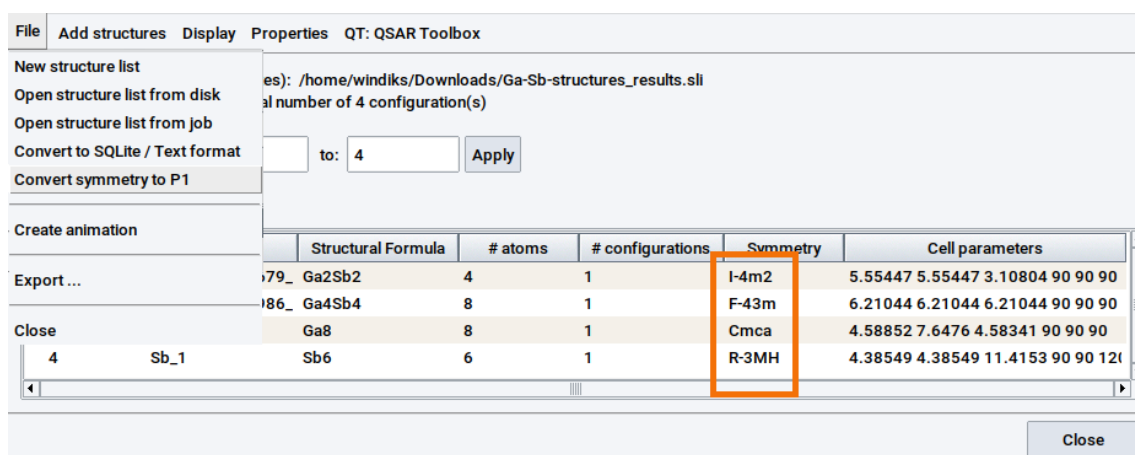


- **New structure list**: Create a new and empty structure list that can be filled with the features of the menu item **Add structures**; the file that stores the structure list should have one of the following extensions: *sli*, *slist*, or *list*

- **Open structure list from disk** : load a file that contains the data of a *MedeA* structure list
- **Open structure list from job** : load a structure list from the currently selected JobServer; the latter is defined via **Jobs** >> **Select server**
- **Convert to SQLite / Text format** : transform the format of a currently opened structure list from the SQLite into a clear text format and vice versa

Hint: By default *MedeA* structure list are stored in the database format SQLite which has the advantage of creating small files, especially, in case of structure lists with several thousand records of data and properties.

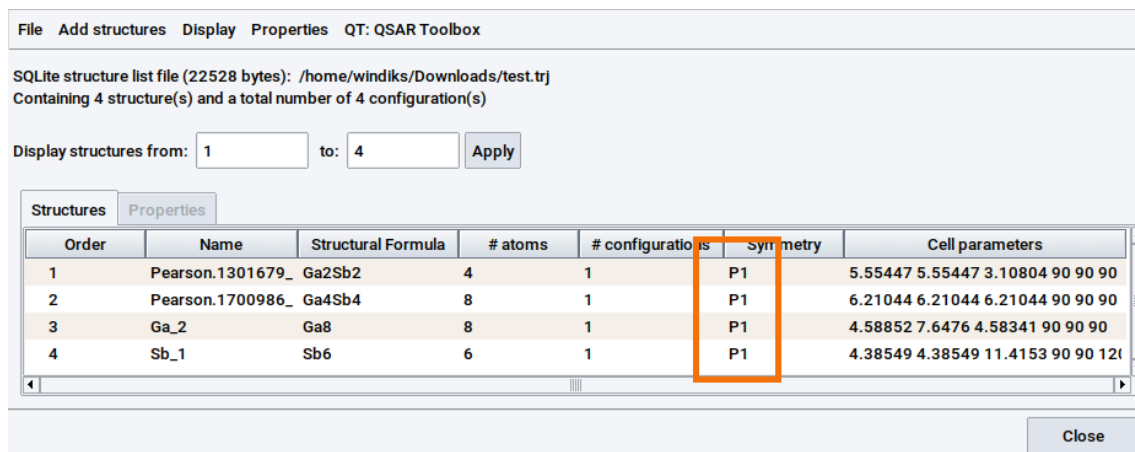
- **Convert symmetry to P1** : Lower the symmetry of all structures of the structure list to the space group *P1*, i.e. remove all point group symmetry operations. With this feature the periodic boundary conditions (PBC) of structures with simulation cells are maintained.



Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
79_ Ga2Sb2	4	1	I-4m2	5.55447 5.55447 3.10804 90 90 90
86_ Ga4Sb4	8	1	F-43m	6.21044 6.21044 6.21044 90 90 90
Ga8	8	1	Cmca	4.58852 7.6476 4.58341 90 90 90
Sb_1 Sb6	6	1	R-3MH	4.38549 4.38549 11.4153 90 90 120



convert symmetry to P1

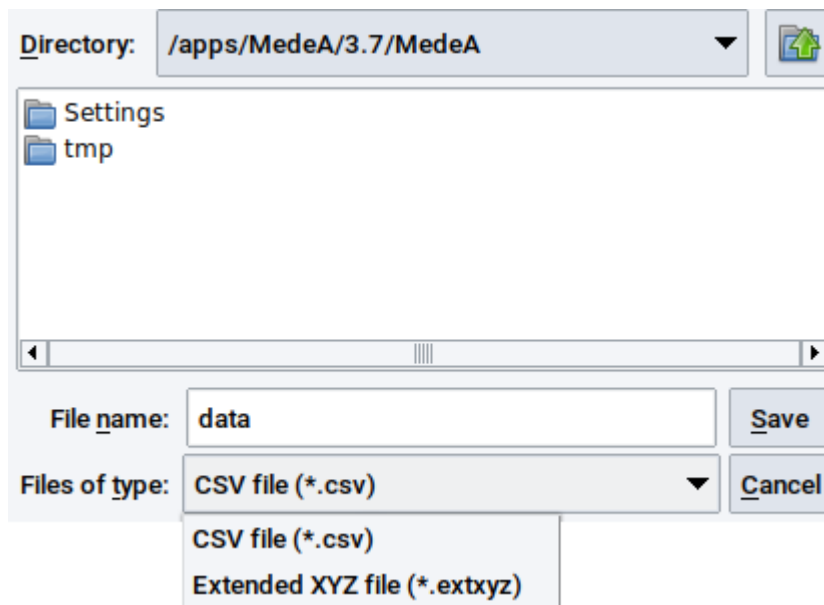


Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	Pearson.1301679_	Ga2Sb2	4	1	P1	5.55447 5.55447 3.10804 90 90 90
2	Pearson.1700986_	Ga4Sb4	8	1	P1	6.21044 6.21044 6.21044 90 90 90
3	Ga_2	Ga8	8	1	P1	4.58852 7.6476 4.58341 90 90 90
4	Sb_1	Sb6	6	1	P1	4.38549 4.38549 11.4153 90 90 120

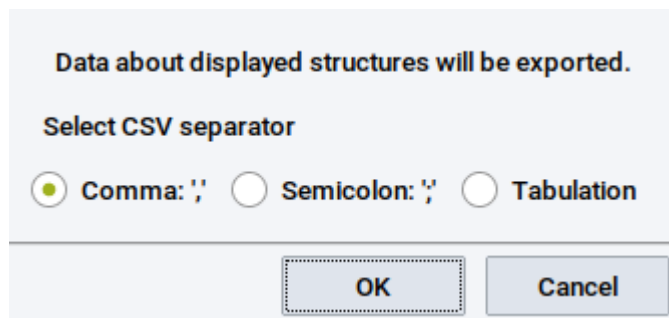
Note: This feature works if the structure list encompasses only the properties that are depicted in the above figure: **Order** , **Name** , **Structural Formula** , **# atoms** , **# configurations** , **Symmetry** , and **Cell parameters**

- **Create Animation** : Animates the structures of the currently open list in an extra animation windows (requires that a structure list is opened and that the structure list contains at least two records)

- **Export...** : Write all the properties that are displayed in the table of the structure list to data file with the extension csv or the structure data in the *extended XYZ* format (extxyz).

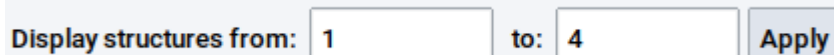


In case you want to save the properties of the table as a data, then first define the filename and then how the values are separated in the data file. The values in the data file can be either separated by commas, semicolons, or tabulators:



- **Close** : Close the structure list and also the structure list editor. A new instance of the structure list editor that is opened via **File** >> **Structure List Editor** does not contain any structure list.

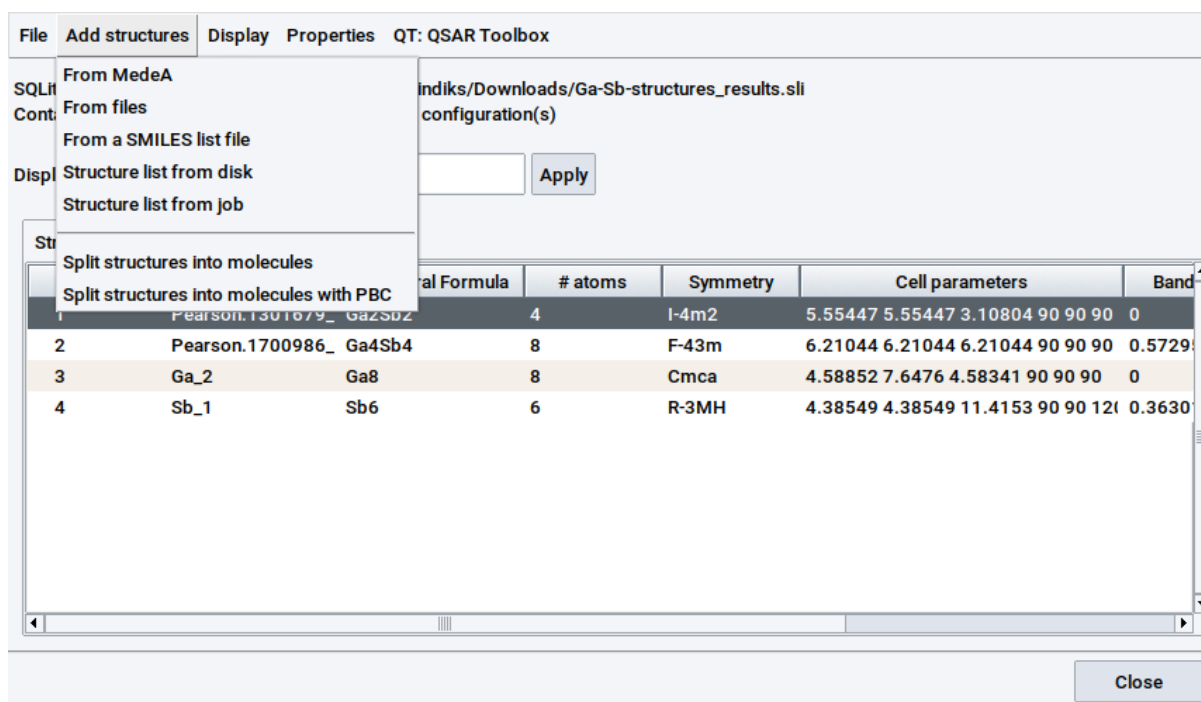
Note: The **Close** button in the lower right corner of the structure list editor has the same effect as the menu item.



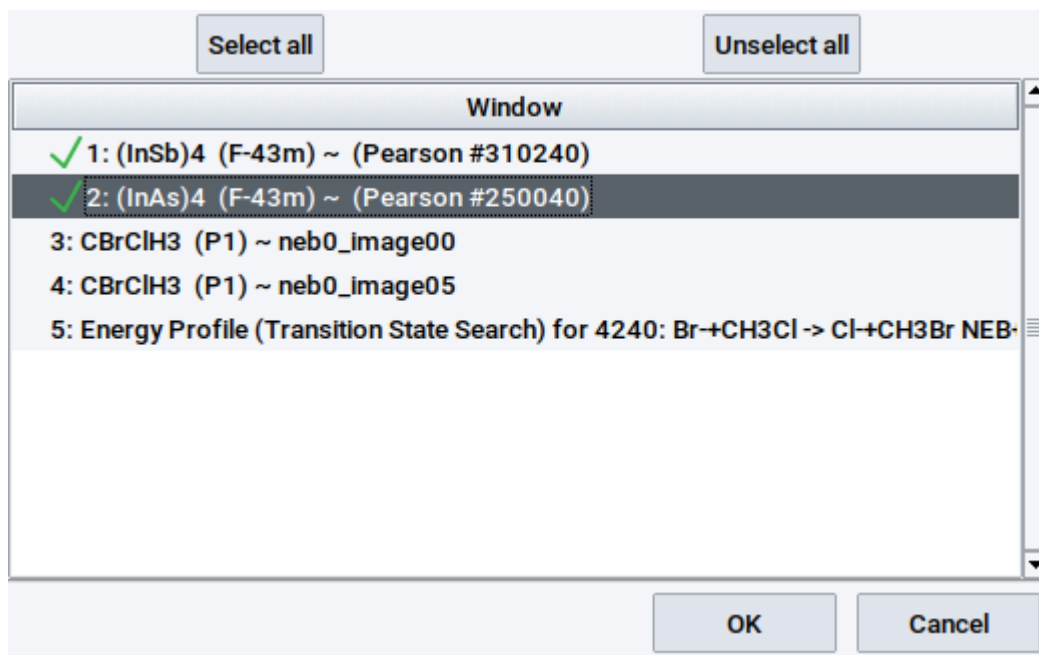
With the options bar **Display structures from: 1 to: 4** **Apply** above the two tabs **Structures** and **Properties** you can define how many structure records of the list are displayed in the structure list editor. After you defined the range with values for **from:** and **to:** confirm the range with **Apply**.

3 Add Structures

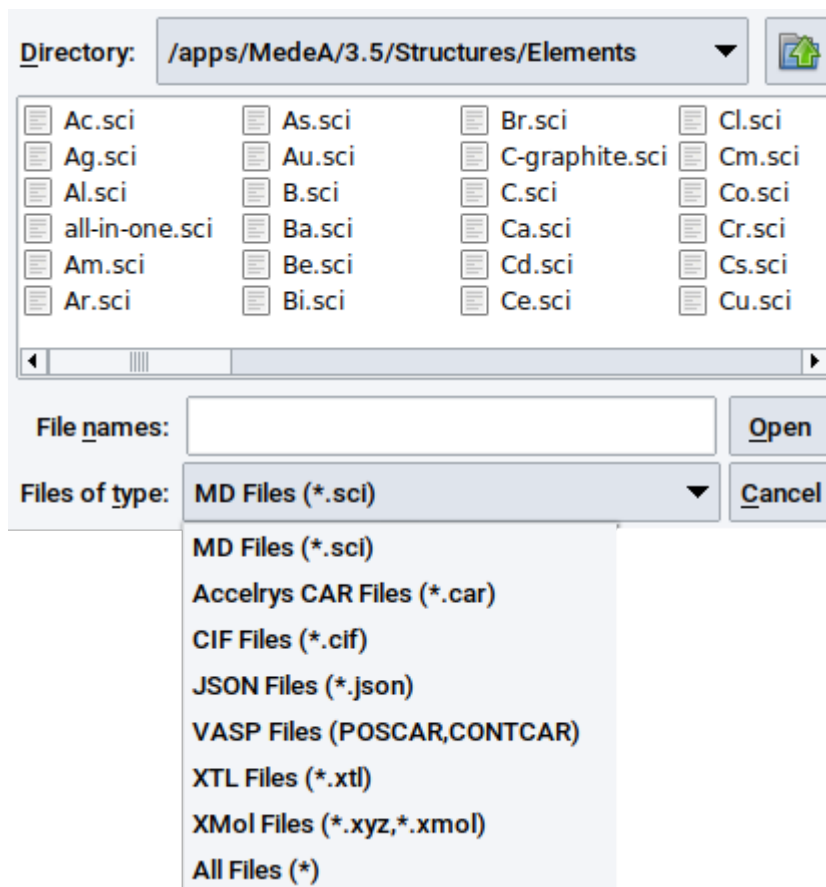
You can add structures via the menu item **Add structures** once a structure list was created or opened with the **File** menu.



- **From Medea** : Add structures that are displayed in the structure windows of the *Medea GUI*



- **From files** : Add structures that are stored in structure data files; supported structure file formats are



- From a SMILES list file :

Use a list of SMILES strings of a file to add molecular structures. The file should contain one SMILES string per line, eventually preceded by a name, e.g.

```

`Alanine  CC(N)C(=O)O`
`Caffeine O=C1C2=C(N=CN2C)N(C(=O)N1C)C`
`Valine  CC(C)C(N)C(=O)O`
`Leucine CC(C)CC(N)C(=O)O`
`Tyrosine NC(Cc1ccc(O)cc1)C(=O)O`
  
```

You can later rename and delete structures from the list and also export all or a selection to individual supported structure data files (1 per structure).

Create molecules:

In periodic box conditions
 as isolated molecules

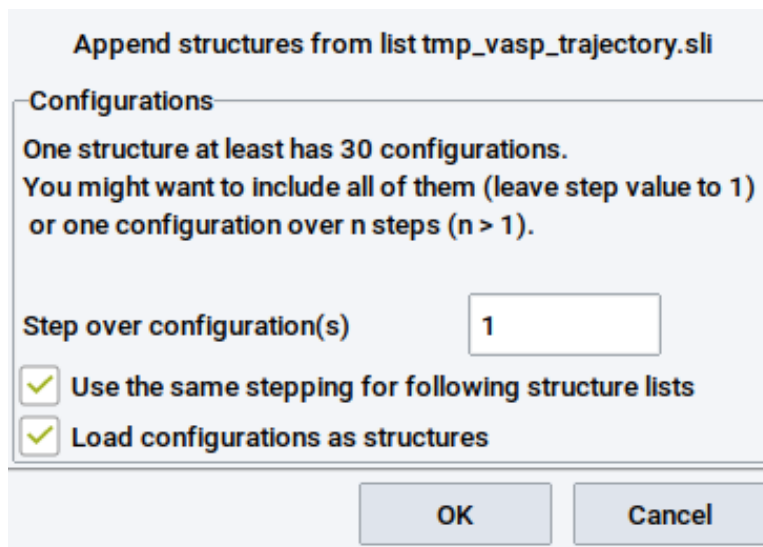
Number of conformers per molecule:

Default 1 means that no search will be done. Depending on the molecule, the number of possible conformers can be smaller than requested. Conformer search strategy will be automatically set according to the molecule connectivity.

With the above dialogue define whether each structure should be an isolated structure (i.e. a molecule in the gas phase) or present in a simulation cell with periodic boundary conditions. Since each structure can have several conformers you can also define how many conformers should be created from each SMILES string.

- Structure list from disk : Add entire *MedeA* structure lists that are stored on disk

- **Structure list from job** : Add entire *MedeA* structure lists that are stored on a selected JobServer. ; the latter is defined via **Jobs** >> **Select server**



Append structures from list tmp_vasp_trajectory.sli

Configurations

One structure at least has 30 configurations.
 You might want to include all of them (leave step value to 1)
 or one configuration over n steps (n > 1).

Step over configuration(s)

Use the same stepping for following structure lists

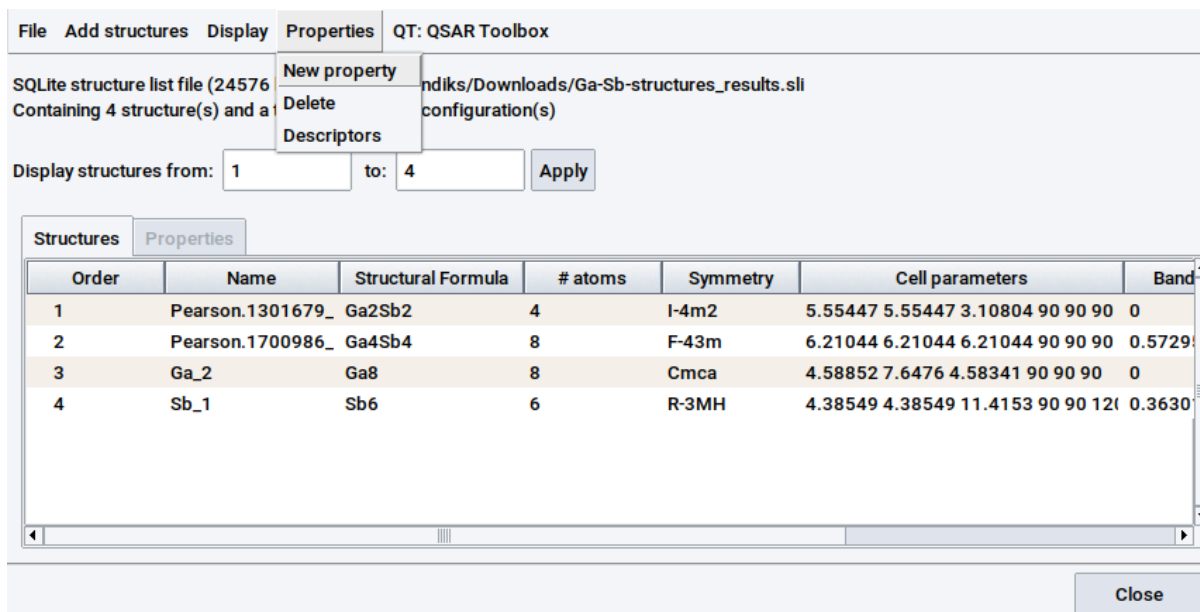
Load configurations as structures

With the above dialogue define if you want to consider each record, every second record, every third record, etc. of the structure list (**Step over configuration(s)**) and whether this stepping should be applied to all imported structure lists, in case you want to import more than one structure list. In case a structure list is a trajectory containing several configurations you can decide whether for each configuration a separate record is created in the structure list.

- **Split structures into molecules** : Add structures that are displayed in the structure windows of the *MedeA GUI*, but split them up in their individual constituents as isolated atoms or molecules, i.e. without periodic boundary conditions (PBC)
- **Split structures into molecules with PBC** : Add structures that are displayed in the structure windows of the *MedeA GUI*, but split them up into their individual constituents in simulation cells with periodic boundary conditions (PBC)

4 Add and Display Properties

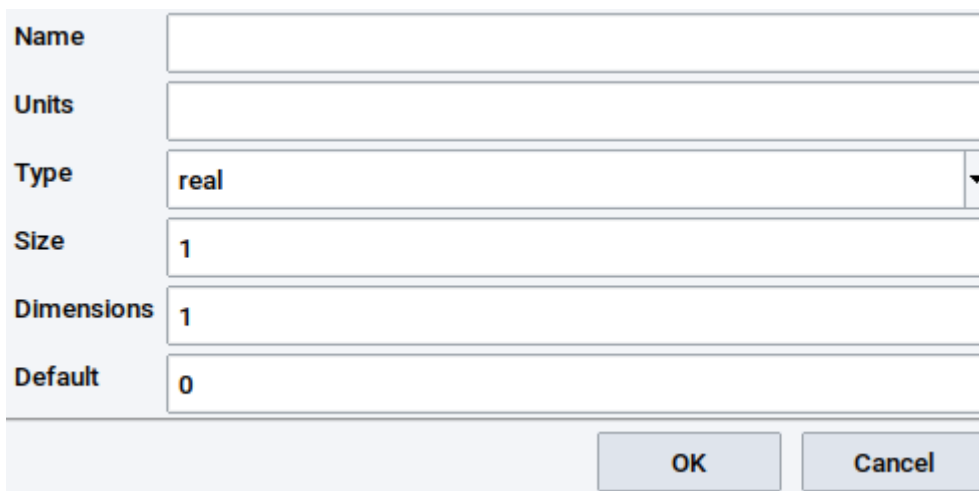
Beside the structural information you can also add properties and structural descriptors to each record of a structure list. One possibility for you is to add properties and their values to an open structure list via the **Properties** menu item:



The screenshot shows the 'Properties' menu open over a table of structures. The table has the following data:

Order	Name	Structural Formula	# atoms	Symmetry	Cell parameters	Band
1	Pearson.1301679_	Ga2Sb2	4	I-4m2	5.55447 5.55447 3.10804 90 90 90	0
2	Pearson.1700986_	Ga4Sb4	8	F-43m	6.21044 6.21044 6.21044 90 90 90	0.5729
3	Ga_2	Ga8	8	Cmca	4.58852 7.6476 4.58341 90 90 90	0
4	Sb_1	Sb6	6	R-3MH	4.38549 4.38549 11.4153 90 90 120	0.3630

- **New property** : Define a new column in the structure list that you can fill with values. With the menu item you bring up the below dialogue:



The dialog box contains the following fields:

- Name**: [Empty text box]
- Units**: [Empty text box]
- Type**: **real** (selected in a dropdown menu)
- Size**: **1**
- Dimensions**: **1**
- Default**: **0**

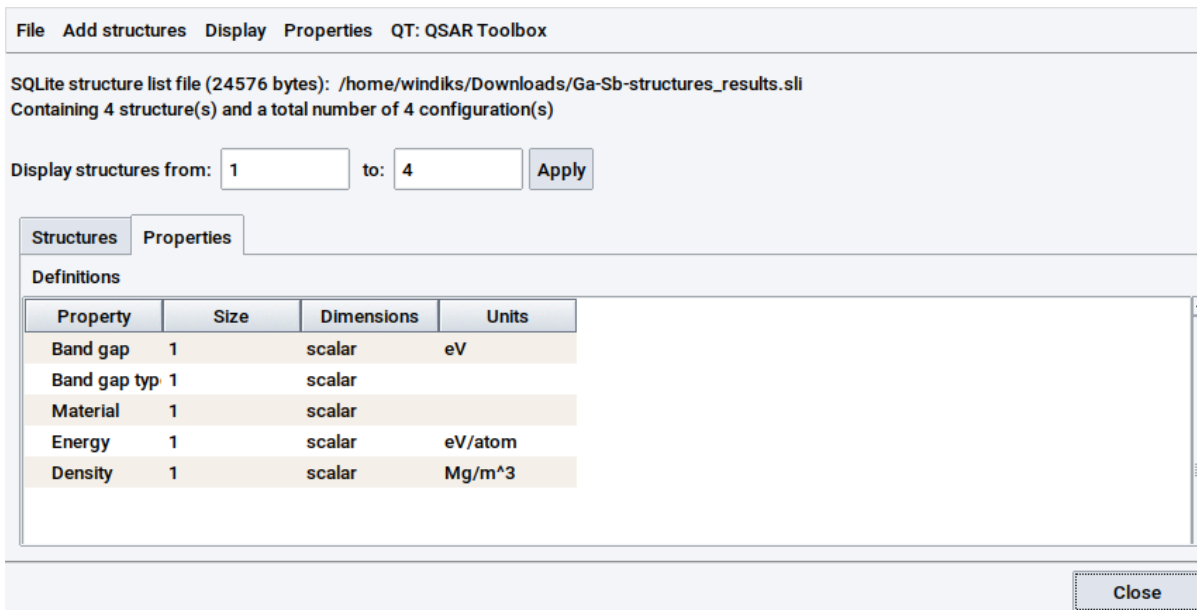
Buttons: **OK** and **Cancel**

- **Name** : Enter a name to appear in the header cell of the column
- **Units (optional)** : The unit of the property
- **Type** : Select from the selection bar **real** for real numbers (default), **integer** for integer numbers, and **string** for text
- **Size** : Define the amount of values for this property; can be 1 (default) or larger
- **Dimensions** the values dimension, e.g. **3 3** means a 3×3 matrix
- **Default (optional)**: The default value to initialize the newly created property column in the structure list; 0 is a reasonable initial value and can be modified afterwards by a double-click in a cell of the table

With the menu sequence **Properties** >> **Descriptors** you add descriptors that are calculated with other properties and/or structural descriptors based on a user-defined equation or correlation. For more information, read the Section HT-Descriptors in which is part of the description of MedeA HT: High Value from High Throughput Simulations.

Hint: This feature requires a separate license for the *MedeA* module *HT-Descriptor*.

Once you have added properties then the **Properties** tab gets accessible. This tab summarizes the name, size, dimension, and unit of each property.



File Add structures Display Properties QT: QSAR Toolbox

SQLite structure list file (24576 bytes): /home/windiks/Downloads/Ga-Sb-structures_results.sli
Containing 4 structure(s) and a total number of 4 configuration(s)

Display structures from: 1 to: 4 Apply

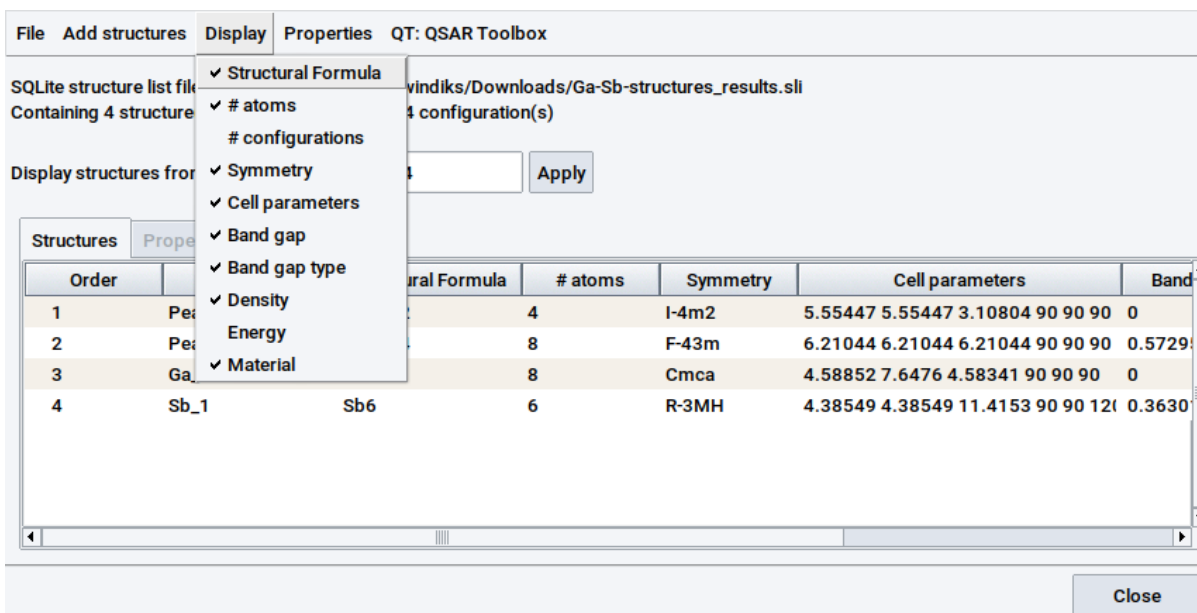
Structures Properties

Definitions

Property	Size	Dimensions	Units
Band gap	1	scalar	eV
Band gap typ	1	scalar	
Material	1	scalar	
Energy	1	scalar	eV/atom
Density	1	scalar	Mg/m ³

Close

To determine which of the columns of a structure list should be shown use the **Display** menu item:



File Add structures Display Properties QT: QSAR Toolbox

SQLite structure list file (24576 bytes): /home/windiks/Downloads/Ga-Sb-structures_results.sli
Containing 4 structure(s) and a total number of 4 configuration(s)

Display structures from: 1 to: 4 Apply

Structures Properties

Display menu items:

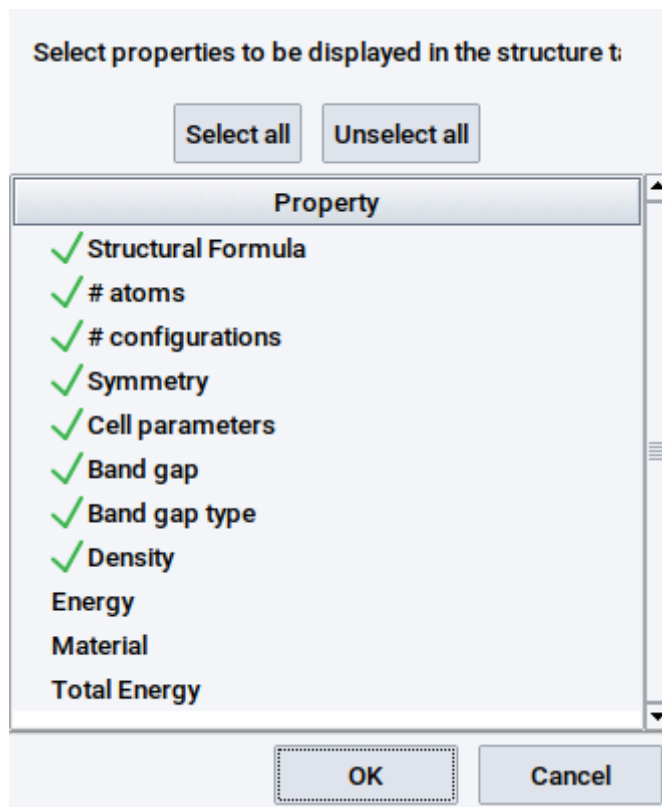
- ✓ Structural Formula
- ✓ # atoms
- # configurations
- ✓ Symmetry
- ✓ Cell parameters
- ✓ Band gap
- ✓ Band gap type
- ✓ Density
- Energy
- ✓ Material

Order	Structural Formula	# atoms	Symmetry	Cell parameters	Band gap
1	Pe	4	I-4m2	5.55447 5.55447 3.10804 90 90 90	0
2	Pe	8	F-43m	6.21044 6.21044 6.21044 90 90 90	0.5729
3	Ga	8	Cmca	4.58852 7.6476 4.58341 90 90 90	0
4	Sb ₁	6	R-3MH	4.38549 4.38549 11.4153 90 90 121	0.3630

Close

A click on a menu item has immediate effect, i.e. either display or un-display a column with a property.

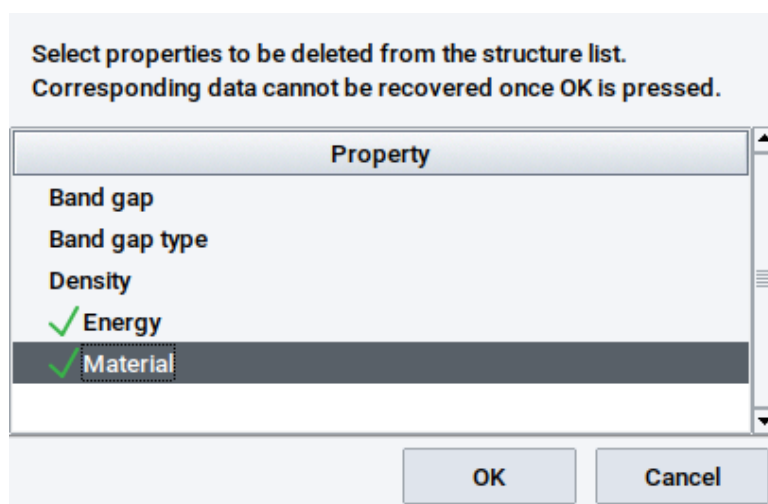
In case a structure list contains more than 10 columns then you can use the menu sequence **Display** >> **Select displayed properties**. That brings up the below dialogue to decide which properties should be shown in the structure list editor.



Click on a row to either add or remove a green check mark; only marked properties are displayed. Confirm your selection with **OK**. Click on **Select all** or **Unselect all** to show all or none, respectively, of the columns.

5 Remove Properties

To delete an entire column with property cells then use the menu sequence **Properties** >> **Delete**. In the below dialogue click on a row to either add or remove a green check mark; only marked properties are deleted.



Confirm your selection with **OK**.

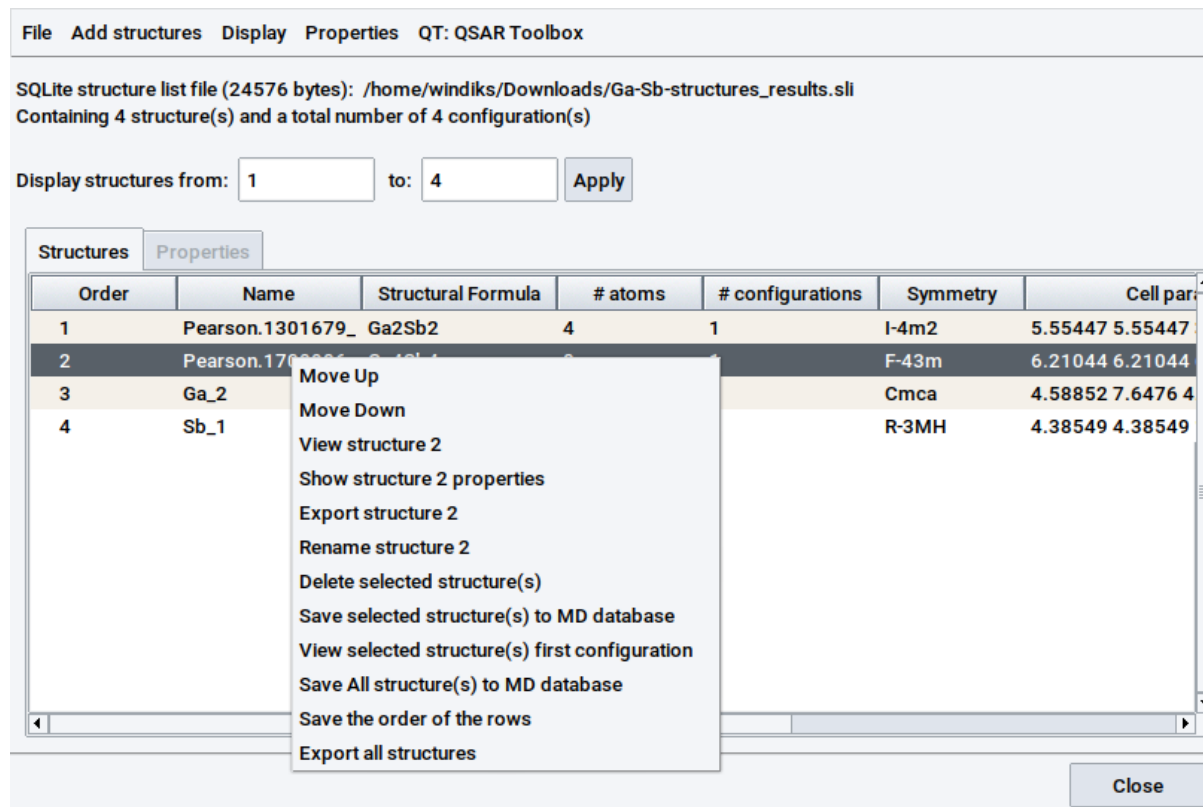
6 Modify List Records

With the context menu of the structure list editor you can modify and manage individual list records or several selected list records. The context menu appears upon right-clicking on a structure list record:

A right-click on one of the data cells (not the header cell!)

- ID
- Name
- Structural Formula
- # atoms
- # configurations
- Symmetry
- Cell parameters

brings up the context menu:



The screenshot shows the MedeA software interface. At the top, there is a menu bar with 'File', 'Add structures', 'Display', 'Properties', and 'QT: QSAR Toolbox'. Below the menu bar, the text reads: 'SQLite structure list file (24576 bytes): /home/windiks/Downloads/Ga-Sb-structures_results.sli' and 'Containing 4 structure(s) and a total number of 4 configuration(s)'. There are input fields for 'Display structures from: 1' and 'to: 4', with an 'Apply' button. Below this is a table with two tabs: 'Structures' and 'Properties'. The 'Structures' tab is active, showing a table with columns: 'Order', 'Name', 'Structural Formula', '# atoms', '# configurations', 'Symmetry', and 'Cell parameters'. The table contains four rows of data. A context menu is open over the second row, listing various actions such as 'Move Up', 'Move Down', 'View structure 2', 'Show structure 2 properties', 'Export structure 2', 'Rename structure 2', 'Delete selected structure(s)', 'Save selected structure(s) to MD database', 'View selected structure(s) first configuration', 'Save All structure(s) to MD database', 'Save the order of the rows', and 'Export all structures'. A 'Close' button is located at the bottom right of the window.

Order	Name	Structural Formula	# atoms	# configurations	Symmetry	Cell parameters
1	Pearson.1301679_ Ga2Sb2		4	1	I-4m2	5.55447 5.55447
2	Pearson.1700000_ GaSb		4	1	F-43m	6.21044 6.21044
3	Ga_2		2	1	Cmca	4.58852 7.6476 4.58852
4	Sb_1		2	1	R-3MH	4.38549 4.38549

A right-click on one of the other cells brings up a context menu with two more items:

File Add structures Display Properties QT: QSAR Toolbox

SQLite structure list file (24576 bytes): /home/windiks/Downloads/Ga-Sb-structures_results.sli
Containing 4 structure(s) and a total number of 4 configuration(s)

Display structures from: to:

Cell parameters	Band gap	Band gap type	Density	Energy	Material
5.55447 5.55447 3.10804 90 90 90	0	no	6.6316	-3.521477	metal
6.21044 6.21044 6.21044 90 90 90	0.572953	direct	5.3005	-2.676522	semiconductor
4.58852 7.6476 4.58341 90 90 90	0	no	5.7		
4.38549 4.38549 11.4153 90 90 120	0.363012	indirect	6.3		tor

Context menu items:

- Paste to Density
- Edit Density value
- Move Up
- Move Down
- View structure 2
- Show structure 2 properties
- Export structure 2
- Rename structure 2
- Delete selected structure(s)
- Save selected structure(s) to MD database
- View selected structure(s) first configuration
- Save All structure(s) to MD database
- Save the order of the rows
- Export all structures

The individual items of the context menus have the following functions:

- **Paste to property** : either enter or replace a value of a property with value stored in the clipboard
- **Edit property value** : modify the value of a cell using the dialogue

Edit structure 1 Band gap value

Property description:
Units: eV Data type: double
Data dimensions: 1 Data size: 1

Value:

Confirm the modification with

Note: Another possibility to modify a value of a property is to double-click in a data cell which makes the content of the cell editable:

File Add structures Display Properties QT: QSAR Toolbox

SQLite structure list file (24576 bytes): /home/windiks/Downloads/Ga-Sb-structures_results.sli
Containing 4 structure(s) and a total number of 4 configuration(s)

Display structures from: to:

ns	# configurations	Symmetry	Cell parameters			Band gap	Band gap type	Den
1		I-4m2	5.55447	5.55447	3.10804	0.572953	no	6.6316
1		F-43m	6.21044	6.21044	6.21044	0.572953	direct	5.3095
1		Cmca	4.58852	7.6476	4.58341	1.2345	no	5.7588
1		R-3MH	4.38549	4.38549	11.4153	0.363012	indirect	6.3799

To confirm the change simply press the **Enter** key of your keyboard.

- **Move Down** : move a row one position **down** (to make this modification permanent use the menu item **Save the order of the rows** of this context menu)
- **Move Up** : move a row one position **up** (to make this modification permanent use the menu item **Save the order of the rows** of this context menu)
- **View structure** : visualize the structure in the *MedeA GUI*
- **Show structure properties** : open the **Properties** tab
- **Export structure** : save this structure to a file on disk in one of the supported formats
- **Rename structure** : change the name of the structure
- **Delete selected structure(s)** : remove the record from the structure list

Hint: Once you click **OK** in the confirmation window then a structure is permanently removed from the list, together with the associated properties. You do not have any possibility to undo this option!

- **Save selected structure(s) to MD database** : create new entries in the *Materials Design Database*, or briefly *MD database* for computed results; this database is searchable with *InfoMaticA*
- **View selected structure(s) first configuration** : visualize only the very first configuration of all selected records in the *MedeA GUI*; this works also if a structure list record comprises one configuration
- **Save all structure(s) to MD database** : create new entries in the *Materials Design Database*, or briefly *MD database* with all structures of the current structure list; the *Materials Design Database* is for computed results and searchable with *InfoMaticA*
- **Save the order of the rows** : make the order of re-arranged rows permanent
- **Export all structures** : save each structure of the current list to separate files on disk in one of the supported formats

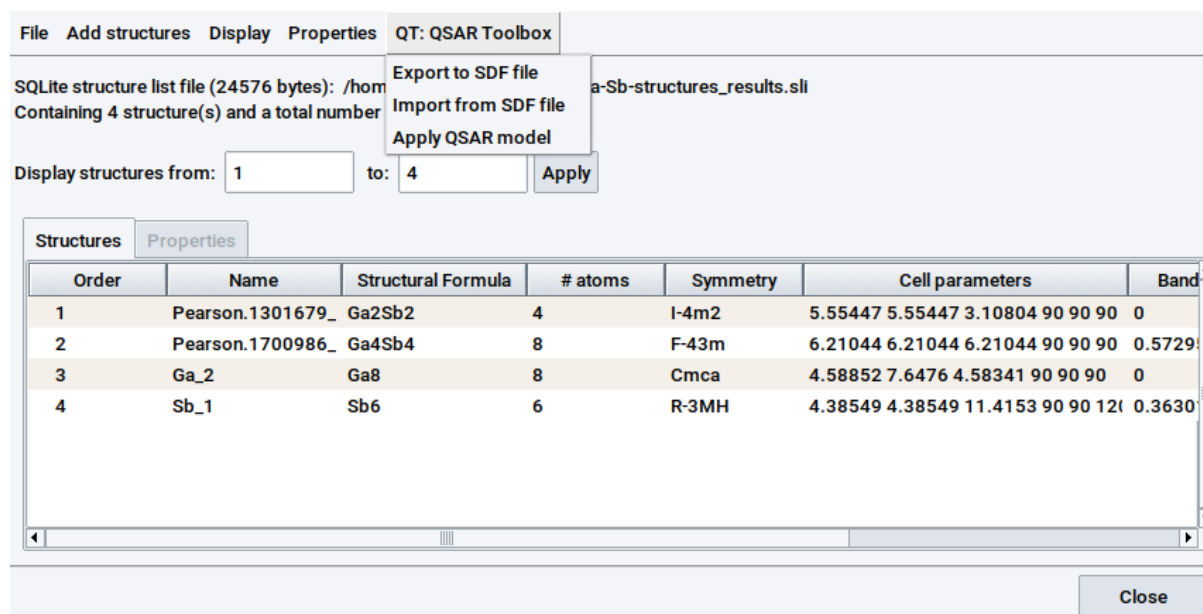
7 Order List Records

Structures are stored in a given order in the list, which appears in the **Order** column in the structures table. It is possible to change the order in the table by sorting rows (structures) according to a column from the right-click context menu commands **Sort Ascending** or **Sort Descending**, on a column title. Also, a given structure can be moved up or down by a right-click on its row with the corresponding command in the context menu.

If the initial order of the rows in the table is changed by one of these methods, the actual structure order in the structure list file remains unchanged. It is possible to apply the new displayed order to reorder the list internal ordering with the right-click context menu command **Save the order of the rows**. This can be useful, for example, to change the order of how structures should be processed in a *MedeA* job.

8 Predict Properties From Correlations

The structure list editor can be used in conjunction with *MedeA QT* to explore and analyze the relationships between descriptors and system properties. In case you have a license for *MedeA QT* then you also see the menu item **QT: QSAR Toolbox**. A click on this menu item opens a pull-down menu that has the items



SQLite structure list file (24576 bytes): /home/.../...-Sb-structures_results.sli
Containing 4 structure(s) and a total number

Display structures from: to:

Order	Name	Structural Formula	# atoms	Symmetry	Cell parameters	Band
1	Pearson.1301679_	Ga2Sb2	4	I-4m2	5.55447 5.55447 3.10804 90 90 90	0
2	Pearson.1700986_	Ga4Sb4	8	F-43m	6.21044 6.21044 6.21044 90 90 90	0.5729
3	Ga_2	Ga8	8	Cmca	4.58852 7.6476 4.58341 90 90 90	0
4	Sb_1	Sb6	6	R-3MH	4.38549 4.38549 11.4153 90 90 121	0.3630

- **Export to SDF file** : Writes to the properties and descriptors to a data file in the *sdf* format, which is readable by *MedeA QT*
- **Import from SDF file** : Reads properties and descriptors from a data file in the *sdf* format
- **Apply QSAR model** : Reads properties and descriptors from a data file in the *xml* format that was created with *MedeA QT*