
# Quick-Start Guide

# SimuLase_TMDC

Version 1.0

**SimuLase_TMDC® for 2D Materials Quick Start Guide**



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## Terminology

SimuLase_TMDC stores all its data in hierarchal structure, referred to in this document as simply a **Database**. A Database is composed of three major components:

**Structure** this file contains all information regarding the layout of the physical device under simulation

**Model** this file contains all information regarding the numerical model used to simulate the structure

**Datasets** a collection of parameterized data files containing computed values

For example, an *Absorption Dataset* contains absorption data for all combinations of parameters requested during a single simulation run. At a minimum a complete database contains four primary datasets named, *Absorption*, *Refractive Index*, *Photoluminescence* and *Band structure*. Additional auxiliary datasets may also be generated depending on the particular configuration of SimuLase model settings.

Key features and capabilities of SimuLase_TMDC include:

- Rigorous and predictive a priori computation key material properties, like, absorption, gain and photoluminescence spectra;
- Poisson solver to compute the influences of dielectric environments due the presence of multiple TMDC layers, substrate- or dielectric coating-materials;
- Physics captured within the relativistic Semiconductor Dirac Bloch model;
- Inclusion of higher order many-body correlations;
- Verified band structure inputs derived from first principles DFT calculations and verified against experimental data;
- Output data can be easily imported into other commercial higher level device software simulation tools.

## Before you Begin

### Installation Requirements

To review complete system requirements and recommendations for your SimuLase software, see the Read Me file included with your software.

### Installing the Software

1 Close any other SimuLase applications open on your computer.

2 Launch the installer (SimuLase.msi) application and follow the on-screen instructions.

### Activate the Software

SimuLase uses license management technology to ensure compliance with the product license agreement. This technology prompts you to verify the license of your product using a 25 character alphanumeric Product Activation Code (example code: `LMP8M-PSDXB-12345-F9BTC-24680`) during the installation process. This code is unique to each installation of SimuLase and is provided to you when the software is purchased.

## Getting to Know SimuLase_TMDC

This Quick Start Guide provides a brief introduction to the key features and capabilities of SimuLase_TMDC as well as a quick tour of its Graphical User Interface. This user interface is designed to reduce clutter, streamline your design process and automats repetitive tasks allowing you to focus on the substance of your design studies. More detailed information, including some work examples, can be found in the companion SimuLase_TMDC User Guide document. Refer to this Users Guide for any feature not outlined in this supplement, or for more detailed information regarding the microscopic modelling of semiconductor devices as implemented in this application.

## Using Online Help

The SimuLase_TMDC Quick Start Guide and the SimuLase Users Guide in PDF format can be accessed through its Help-menu on the Main menu bar. Additional information, including the most up-to-date version of all documents, can be downloaded from www.nlcstr.com

## Design, Simulate, Analyze

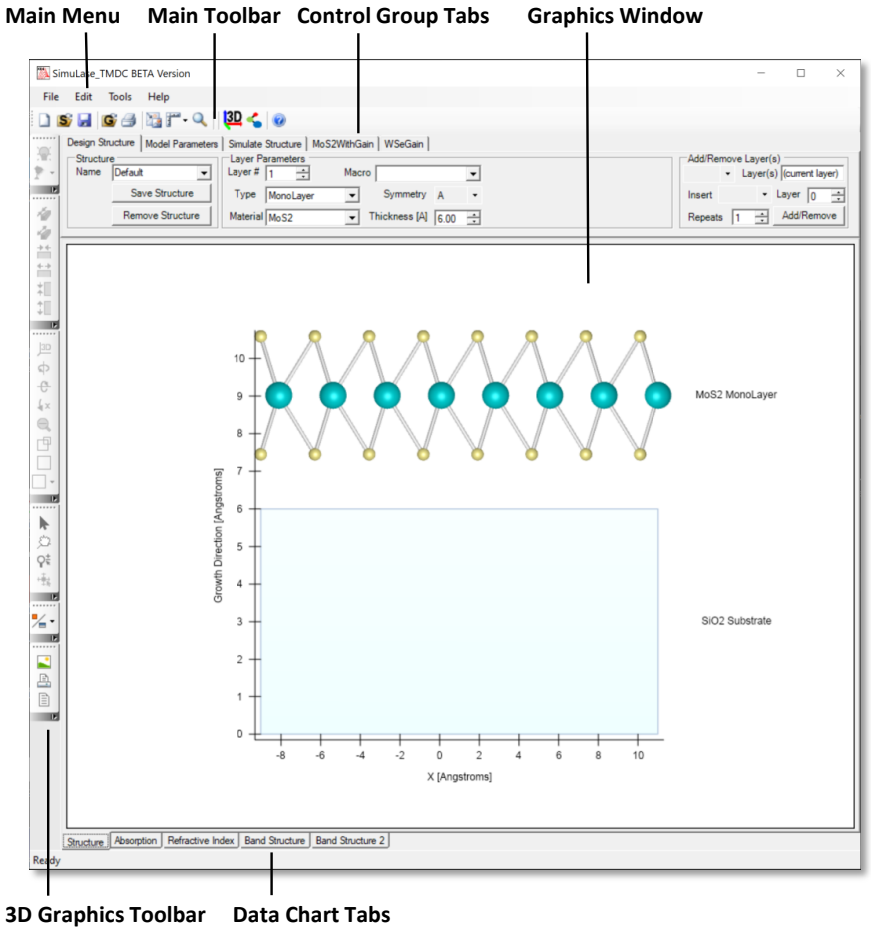



Figure 1 The Main Screen showing the control layout

SimuLase_TMDC is designed around a three-stage workflow.

1) *Design the structure*: Using the layer designer the user interactively stacks layers of different materials to produce a layered structure device.

2) *Simulate the structure*: The structure is simulated using:
    a. Numerical Model parameters are selected that specify the resolution and complexity of the microscopic many-body model.
    b. Computational parameters that dictate the amount of computational resources allocated, (i.e., number of CPU cores) and parameter ranges over which the structure is simulated – like, e.g., carrier densities or temperatures.

3) *Analyze the structure*: Numerical results generated by the simulation are loaded and rendered in a series of charts. Results from previously executed simulations may also be loaded for comparative analysis. Interactive tools are provided in each chart to facilitate analysis and annotation of data charts. Raw and post processed datasets and publication quality plots may be exported in standard formats.

The SimuLase Graphical User Interface (GUI) implements each stage of this workflow by grouping controls related to each stage in separate tabbed windows. The following is a brief description of the main functionality of the each component of the SimuLase User Interface.

After starting SimuLase_TMDC, various controls are shown at the top of the application window. The controls are organized in three tabs labeled **Design Structure**, **Model Parameters** and **Simulate Structure**. In a typical workflow the user will move from left to right, sequentially clicking each tab and interacting with the controls. Below the control tabs is the main graphics window showing the current device structure. After simulating a structure, a number of additional tabs appear below the main graphics display. These tabs are used to switch between displays of the various datasets generated during the simulation.

## Design a Structure

The controls on the **Design Structure** tab, located above the main graphics window, are used during construction of a layered device and dynamically view and modify all aspects of the resulting device structure. The **Graphics Window** can display 2D or 3D interactive renderings of the layered device as it is constructed.

### Selecting, Adding and Removing Layers

Layers are added or removed from the structure by *left-clicking* the mouse anywhere on the structure. The selected is indicated by adding a dashed black line around the perimeter. A context menu will appear which contains options to remove the selected layer or add a new layer. Adding a new layer will add a new $MoS_2$ layer to the top of the structure. This newly added layer may be modified by selecting the new layer and using the controls on the Design Structure tab to change the layer Type (Monolayer, HetroBiLayer Bulk or DFT_MDF) and the layer material from the Material pulldown.

The current structure can be cleared by clicking on the **Remove Structure** button on the on the Design Structure tab. This deletes the current structure from SimuLase allowing the user to construct a new structure. The first layer added to a new structure will automatically be chosen to be a Silicon dioxide ($SiO_2$) substrate layer and the second layer added will be a layer of $MoS_2$. The material composition of any layer may be modified by the user after it is placed on the canvas.

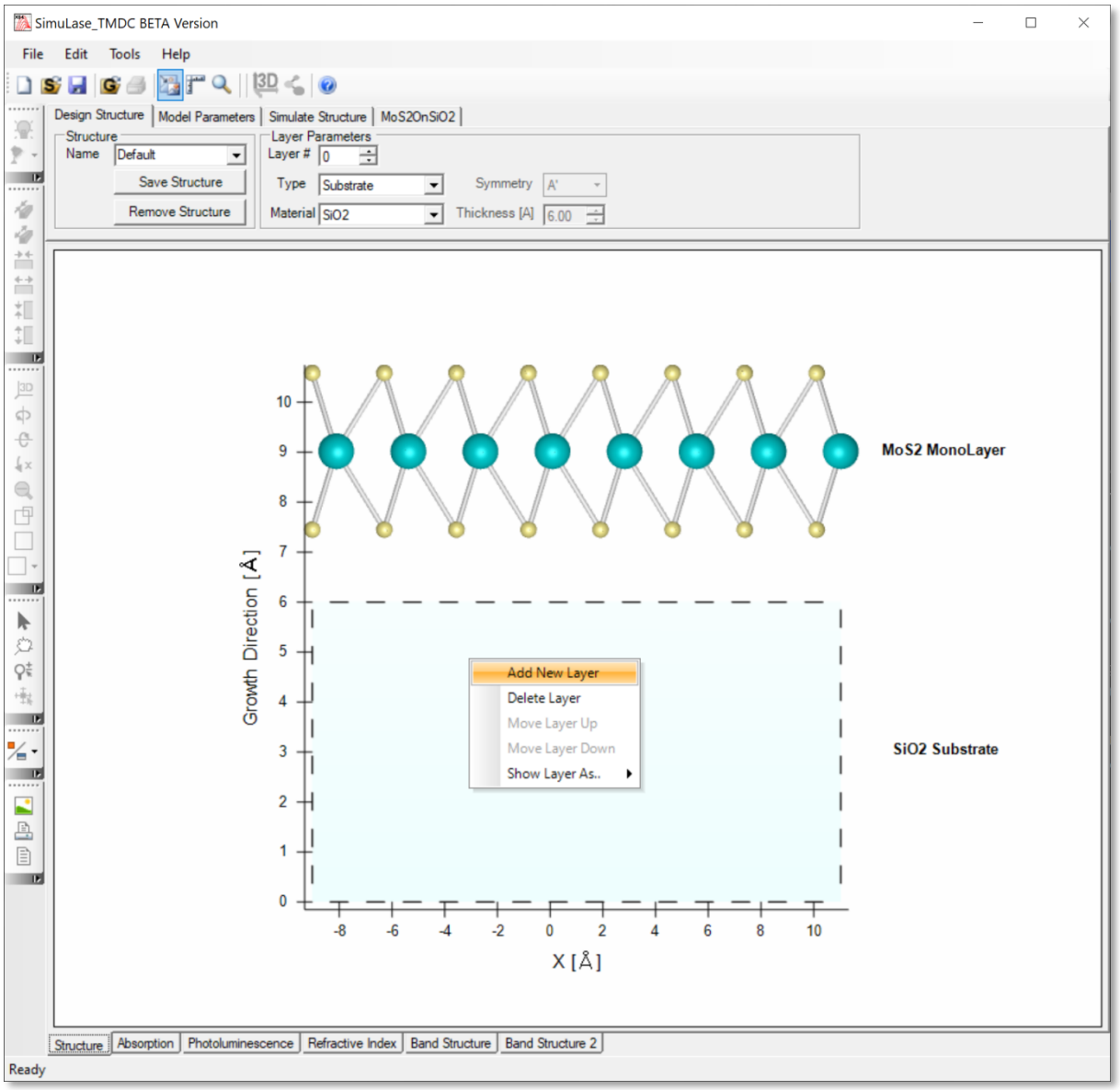



Figure 2 Selecting and Adding or Removing layers using the mouse context menu

The **Design Structure** tab is the default tab that appears when SimuLase is started. The default graphics window tab displays a basic 2-layer structure consisting of a Molybdenum disulfide ($MoS_2$) monolayer on a Silicon dioxide ($SiO_2$) substrate layer. The default structure may be replaced by selecting **File | Open Structure...** from the main menu to load a previously stored structure from disk.

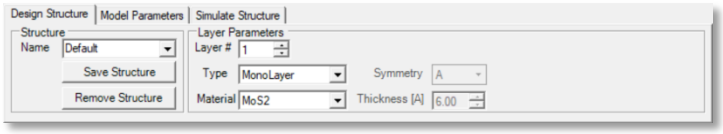



Figure 3 The Design Structure Controls

The controls on the **Design Structure** tab are arranged into two functional groups that provide the following functionality:

**Structure** controls for naming, Saving and Removing the entire structure;
**Layer Parameters** controls for viewing and editing of the properties of a single layer;

The individual controls in each of these functional groups are detailed in the following sections.

## Structure

The controls in this group relate to the overall structure. They are used to attach a unique identifying name to the structure, save the structure to disk or remove the entire structure from memory.

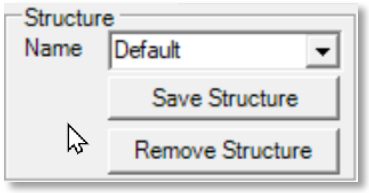



Figure 4 The Structure Controls

**Name** is a string use to describe the entire structure. The structure name is initially assigned the name "Default" but should be changed by the user for each new structure. It is used throughout SimuLase to uniquely identify the structure. The name is prepended to all data files that are generated when the structure is simulated. When multiple Databases are loaded into SimuLase, for data analysis and comparison, all loaded structures are listed in the **Name** pulldown, the user may select which structure is rendered in the Structure window be selecting the appropriate name from the list.

**Save Structure** Information describing all aspects of the current structure is saved in a *SimuLase Structure File* (*.sls) using the structure name as the filename and the three letter extension **.sls**. The file is saved in ASCII using standard human readable xml-format. These files can be read using an external viewer or editor application such as, Microsoft Word, Microsoft Excel, Notepad or any Web Browser. While it is possible to edit this file in an external editor, great care should be taken as it may result in an invalid file when read back into the SimuLase GUI.

**Remove Structure** Deletes the currently loaded structure from SimuLase allowing the user to construct a new structure.

## Layer Parameters

The various controls in this group are used to display and edit the physical properties of the currently selected layer. Changing any of the displayed values for the current layer will cause the corresponding layer in the structure to be updated.

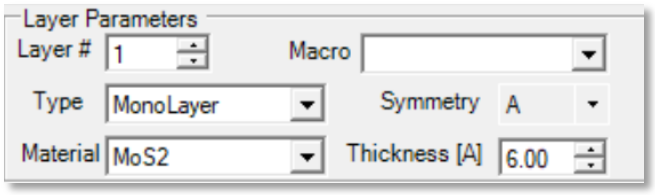



Figure 5 The Layer Parameters Controls

**Layer#** A single layer is selected by changing the number field in this control (or using the mouse to select the layer by clicking anywhere on the layer shown in the graphics window). Layers are numbered sequentially starting with layer 0. The graphics window highlights the currently selected layer by surrounding the layer with a thick dashed line around the layer perimiter.

**Type** A descriptor of the type of layer in the structure. A layer can be one of five types, *Substrate*, *MonoLayer*, *Hetero-Bi-Layer*, *Bulk or DFT_MDF*.

- *Substrate* is either a metal or dielectric material. Its thickness is assumed to be infinite below or above the active TMDC material. Only the dielectric properties of the material are taken into account in evaluating the screening of the Coulomb interaction of the TMDC material. NLCSTR will add additonal Substrate materials on demand at no cost to the user.
- *Monolayer* is a single layer of TMDC material. Several *Monolayers* of the same material can be stacked to form a homo-multi-layer structure.
- *Hetero-Bi-Layer* is a set of two monolayers of different TMDC materials stacked on top of each other. In contrast to a homo-multi-layer structure, this configuration requires additional material paramters specifying the band offsets between the two materials.
- *Bulk* is bulk TMDC material. For this case potentially present *Substrate* layers are not taken into account in the calculation. The calculation is performed using the same material parameters as for a monolayer but replacing the dielecrtic evironment by that of the bulk TMDC material.
- *DFT_MDF* is a user-defined material for which the user provides all relevant material parameters as obtained through DFT calculations. The determination of material parameters from the output of VASP calculations is aided by the **DFT_to_MDF** tool under the **Tool** pull-down menu. For a description of the details of the implementation of a user define DFT material see the corresponding section of the user manual.

**Materia**l The material composing the layer.

**Symmmertry** This field is currently disabled. In future versions of SimuLase_TMDC, this field will allow to select between A- and B-type stacking-orders of TMDC monolayers.

**Thickness [A]** The thickness of the current layer in Angstroms. This field is currently disabled and is automatically set from data contained in the material database,. In future versions of SimuLase_TMDC this field will allow to specify the thickness of *Substrate*-type layers, like, e.g., air or dielectric coatings, which can be located between layers of TMDC material.

## The Graphics Window

The **Graphics Window** is used to display the current structure or line plots of the datasets produced after executing a simulation of the structure. A series of tabs along the bottom drawing area are used to select between the various types of data that can be rendered on the drawing canvas.

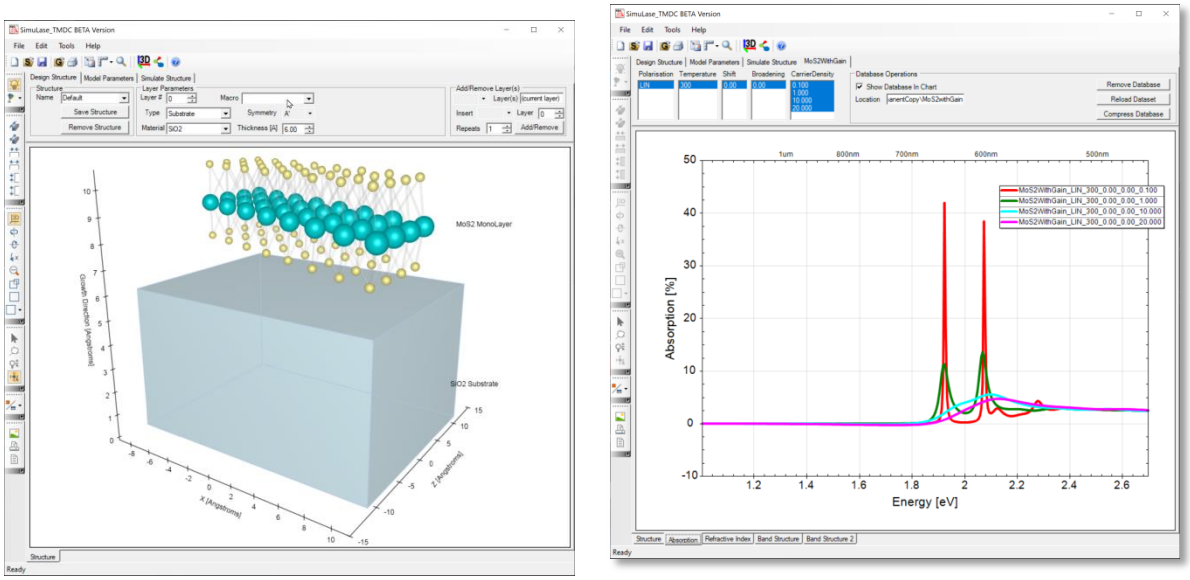



Figure 6 The Graphics Window

As shown in Figure 6 (left), when the **Structure** tab at the bottom of the graphics window is selected a 2D or 3D interactive rendering of the current layer device is displayed. After simulating a structure, or loading in precomputed results from a previous simulation, a number of new tabs are added to the bottom of the graphics window. Selecting one of the tabs causes the relevant data to be rendered to the graphics canvas. For example Figure 6 (right) shows line plots of the Absorption data for the Molybdenum disulfide ($MoS_2$) monolayer on a Silicon dioxide ($SiO_2$) substrate layer structure shown in Figure 6 (left).

## Simulate a Structure

Simulating a structure involves setting controls on the tabs **Model Parameters** and **Simulate Structure**. The Model parameters tab contains controls that specify the resolution and complexity of the model. The Simulate Structure tab contains controls that allow the user to specify a range of parameters, such as polarizations, temperatures, carrier densities for which the structure is

simulated. It also shows the available computational resources and allows the user to dictate the number of CPU cores allocated to the simulation.

## Model Parameters

The controls on the **Model Parameters** tab are arranged into four functional groups that provide the following functionality:

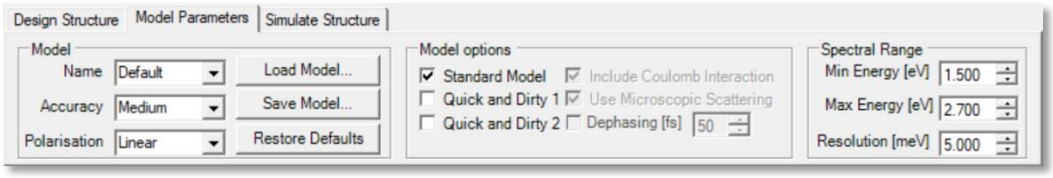



Figure 7 Model Parameters

**Model** controls that deal with the model such as a name for the model and saving and loading pre-defined models.

**Model Options** controls the microscopic model for simulating structures. The default is the

*Standard Model* which includes all Coulomb effects and microscopically calculated electron-electron and electron-phonon scatterings.

*Quick and Dirty 1* includes excitonic effects on the Hartree-Fock level but replaces the dephasing causing scatterings by a simple dephasing time, $T_2$.

*Quick and Dirty 2* neglects all Coulomb effects and performs a simple single-particle calculation on the level of Fermis Golden Rule.

**Spectral Range** controls the spectral range for which spectra shall be calculated. Default values that cover the spectral range of highest interest are set automatically for all materials that are implemented in SimuLase_TMDC. The user can use these controls to refine the resolution, expand or reduce the spectral range and to set these parameters for user defined DFT_MDF materials.

The individual controls in each of these functional groups are detailed in the following sections.

### Model

The controls in this group relate to the overall structure. They are used to attach a unique identifying name to the structure, save the structure to disk or remove the entire structure from memory.

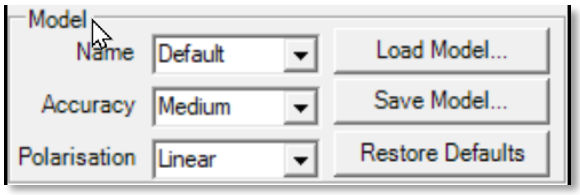



Figure 8 Model Options

**Name** is a string use to describe the collection of model parameters. The model name is initially assigned the name "Default" but should be changed by the user for each new model configuration created. It is used in SimuLase to uniquely identify the collection of model parameters. The name is employed when the same structure is modeled using a different set of parameters.

**Accuracy** accuracy can be set to *High*, *Medium* or *Low* and determines the number of momentum grid points used in the simulation and, thus, the accuracy of the calculations. The calculation time and CPU-memory requirement scale strongly with the accuracy level. Typicaly, the calculation time increases by about a factor of four when going to a higher accuracy level. By default the accuracy-level is set to *Medium* which we recommend for typical calculations.

**Polarization** sets the light-polarization for which the spectra will be calculated to Linear, Circular -L (left circular) or Circular-R (right circular). The calculation time is independent of the choice of polarization.

**Save Model** Information describing all aspects of the current model is saved in a *SimuLase Model File* (*.slm) using the model name as the filename and the three letter extension **.slm**. The model parameters file is saved in ASCII using standard human readable xml-format. These files can be read using an external viewer or editor application such as, Microsoft Word, Microsoft Excel, Notepad or any Web Browser. While it is possible to edit this file in an external editor, great care should be taken as it may result in an invalid file when read back into the SimuLase_TMDC GUI. A .slm file is also created by each simulation with the prefix as specified for the database.

**Load Model** Information describing all aspects of the current model is loaded from a preexisting *SimuLase Model File* (*.slm). All existing model parameter values in the GUI are erased and replaced with the corresponding values in the loaded model file.

**Restore Defaults Model** All existing model parameter values in the GUI are erased and replaced with default values.

## Model Options

The controls in this group specific the global behavior of the backend numerical calculation.

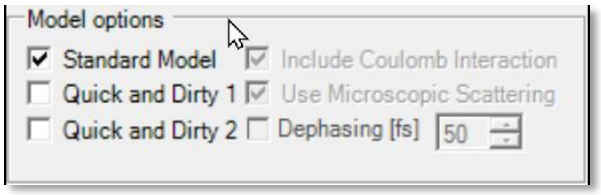



Figure 9 Model Options

**Standard Model** by checking this option, the recommended fully microscopic model for calculating reliable Gain Databases is selected. This is the most extensive model available, including all Coulomb effects and microscopically calculated electron-electron and electron-phonon scatterings that are required for correct lineshapes and amplitudes.

**Quick and Dirty 1** by checking this option the GainDatabase is set up using a model that includes everything the *Standard Model* (above) takes into account except for microscopic scatterings and higher order excitonic correlations which are source terms for the PL. Since the scatterings are not used to describe the dephasing of the optical polarization, a dephasing time *Dephasing* has to be used. Calculation times within this model are much shorter than when using the the *Standard Model* However, the resulting lineshapes, spectral positions and amplitudes will have significant errors. The calculations lose their quantitatively predictive quality that the *Standard Model* provides. The resulting radiative carrier lifetimes are typically wrong by a factor of five or more.

**Quick and Dirty 2** by checking this option the least computationaly intensive model will be used in the simulations. In addition to the simplifcations used by option 'Quick and Dirty 1', this model also neglects all Coulomb effects, including excitons and bandgap renormalizations. It requires the user to specify a value for Dephasing time. With these simplifications the calculation time for one carrier density and one temperature usually reduces to a few seconds. This option can be used to quickly get some very rough estimates or to check the influence of Coulomb effects by comparing to the more sophisticated models.

**Include Coulomb Interaction** if this option is not checked, all Coulomb effects are neglected, including all microscopic scatterings and higher order excitonic correlations. Unchecking this option reduces the model to the level of *Quick and Dirty 2* described above. If un-checked, a dephasing time $T_2$ has to be specified.

**Use Microscopic Scattering** if un-checked, the dephasing of the optical polarization will be described by a dephasing time, $T_2$, rather than by calculating the underlying electron-electron and electron-phonon scattering processes.

**Dephasing Time** if checked, the specified dephasing time will be used for the dephasing of the optical polarizations. This usually leads to significant errors in the lineshapes, amplitudes and spectral positions. Even if microscopic scatterings are taken into account, this dephasing time is added into the description of the dephasing of the polarizations unless this field is un-checked or deactivated.

### Spectral Range

The controls in this group set the spectral range for which spectra shall be calculated. By default these values are set to a 'reasonable' estimate according to the bandstructure of the TMDC materials.

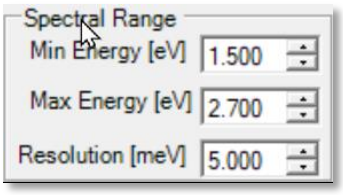



Figure 10 The Spectral Range and Resolution Controls

**Min Energy** sets the lowest transition energy, in electron Volts, for which spectra shall be calculated. By default, this is set to be about 0.5 eV below the A-bandgap.

**Max Energy** sets the highest transition energy, in electron Volts, for which spectra shall be calculated. By default, this is set to be about 0.5 eV above the B-bandgap.

**Resolution** sets the spectral resolution, in meV . By default this is set to 5 meV. For spectra with sharp features this should be reduced. The calculation time scales about linearly with the inverse of the resolution.

## Simulate Structure

The controls on the **Simulate Structure** tab are arranged into two functional groups that provide the following functionality:

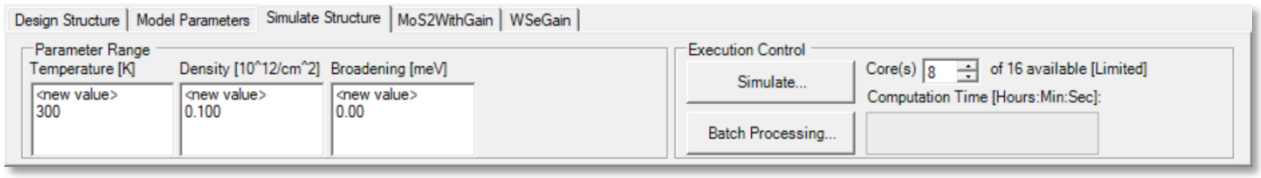



Figure 11 The Simulate Structure Controls

**Parameter Range** used to specify the parameters for which the backend numerical simulator will produce datasets;
**Execution Control** controls relating to the launching and execution of structure simulations;

The individual controls in each of these functional groups are detailed in the following sections.

### Parameter Range

The controls in this group relate to the overall structure. To enter a value to the list double-click on *'<new value>'*, replace the string by a number and hit return to confirm. To delete an entry double click on it, hit the *'backspace'* or *'delete'* button and then *'return'* to confirm. Data will be calculated

for all possible combinations of temperatures, densities and inhomogeneous broadenings. The calculation time and amount of produced data scales with the number of entries in the 'Temperature'-field times the number of entries in the 'Density'-field. The number of broadenings has virtually no influence on the calculation time. However, the amount of produced data increases linearly with the number of broadenings which might have be considered if very large number of datasets are to be created.

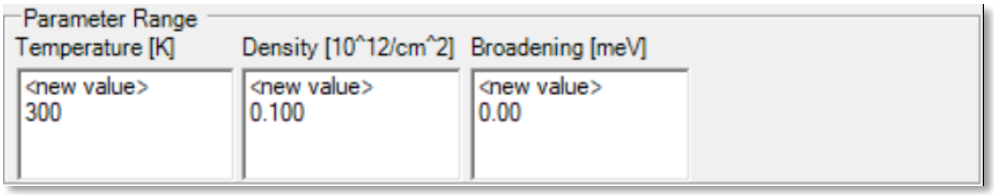



Figure 12 Parameter Ranges

**Temperature** [K]: sets up a list of temperatures in Kelvin for which the database shall be created. The temperature as entered here is used as lattice and carrier temperature. The calculation effort increases with decreasing temperature as higher momentum grid resolution is required due to increased spectral sharpness at lower temperature.

**Density** sets up a list of electron sheet carrier densities in units of [$10^{12}$/cm$^2$]. It is assumed that the carriers are in thermal equilibrium. Currently SimuLase_TMDC assumes an equal electron and hole carrier density and each is given by the values as specified here.

**Broadening** Sets up a list of inhomogeneous broadenings in units of [meV] (FWHM). Besides the spectra that include only the homogeneous broadening due to electron-electron and electron-phonon scattering, inhomogeneously broadened copies of the spectra will be generated.

## Execution Control

The controls in this group relate to the launching of a calculation of the structure using to the model parameters that have been set in the Parameter Range control group. After the *Simulate* button is clicked a file manager window opens to specify a name for the database and the directory into which it shall be written. In case of computations that require significant CPU memory your computer will be mostly unusable for other purposes. Using the computer for other purposes while a database is created can cause problems to the calculation. On a multi-processor machine one should leave at least one processor open for alternative work.

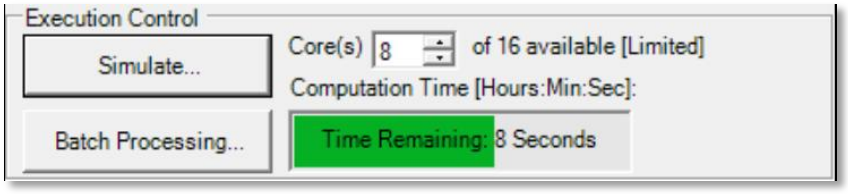



Figure 13 Execution Control

**Simulate** clicking this button starts the calculation of the structure using to the model parameters.

**Core(s)**: defines the number of processors that will be used for the calculations. Creating the data for each temperature-density combination is done sequentially but the calculation is parallelized over the number of processors as defined in the '*Core(s)'* control.

**Progress Bar** this control displays information regarding the progress of the simulation and the aproximate time remaining.

**Batch Processing** this control is currently disabled. In future versions of SimuLase_TMDC it will allow to batch-process variations of parameters other than those as specified on the field *Parameter Ranges*, like dielectric layer widths or MDF parameters of user defined *DFT_MDF* materials.

## Analyze Results

Numerical results generated by the simulation are loaded and rendered in a series of line charts displayed in the Graphics Window. Results from previously executed simulations may also be loaded for comparative analysis. Interactive tools are provided in each chart to facilitate analysis and annotation of data charts. Raw and post processed datasets and publication quality plots may be exported in standard graphics file formats.

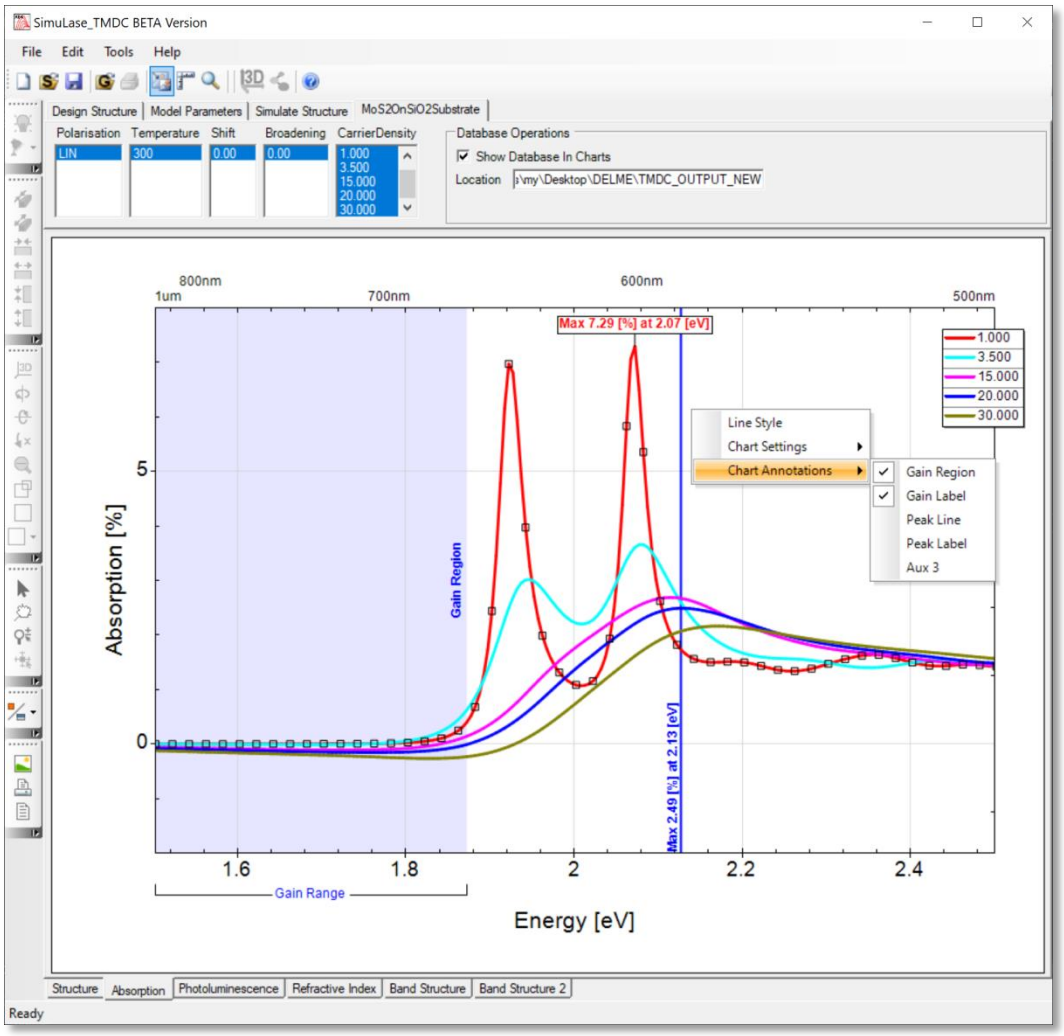



Figure 14 A typical view of SimuLase_TMDC while analyzing data

## Loading and Interacting with Databases

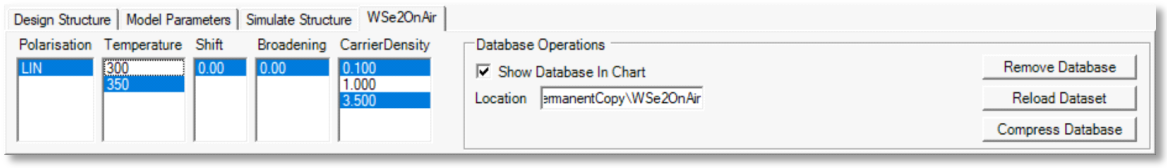
Multiple databases may be loaded into SimuLase_TMDC. After running a simulation, the newly created database is automatically loaded. A preexisting database can be loaded into SimuLase by selecting **File | Open Gain Database...** or using the Open Database icon .

After loading a database, a new tab containing the database name is added to the Control Group Tabs near the top of the screen. A new chart tab for each of the primary datasets (Absorption, Photoluminescence etc.,) is added to the chart tabs along the bottom of the graphics window. All currently loaded databases are plotted in same chart, for example the Absorption Chart can display absorption data from all currently loaded databases. This enables comparative analysis of datasets from different simulation databases.

Dataset plots are accessible via a series of tabs along the bottom of the Graphics Window. By selecting the appropriate tab, a user can view line plots of the main simulation result datasets i.e. 'Absorption', 'Photoluminescence' (i.e. Spontaneous Emission) and 'Refractive Index'.

### Interacting with Datasets

When a database is loaded, a new tab bearing the name of the database is added to the Control Group Tabs above the Graphics Window. The controls on this tab select which data series from the database are plotted in the various charts, and perform various operations on the database.




The tab shows lists of all parameters contained in the database. The user may select a subset of parameters by left-clicking the mouse on the entries in the parameter lists. At least one entry in each parameter list must be selected. A single mouse click within the list will select that single parameter value. Multiple disjoint parameters may be selected by pressing the CTRL key while clicking entries in a parameter list. A continuous range of parameters may be selected by clicking on a value, and then pressing the SHIFT key while clicking on another parameter in the same list, all parameter values between the two clicked values will be selected. In all cases the data displayed in all charts will be immediately updated to display line plots of the selected parameter combinations.

### Database Operations

The controls in this group are used to perform various operations on a whole database.

**Show Database In Chart** If this control is checked, the selected parameter sets will be plotted in the chart window. This is primarily of use when multiple databases have been loaded for comparative analysis. The user may dynamically Show or Hide line plots from the database in the chart window.

**Location** Shows the location of the database on disk. If the full pathname to the database is too long to fit in the location window, moving the mouse pointer into next window will cause a temporary panel to pop showing the entire pathname.

## Interacting with Charts

Charts in SimuLase are configurable in terms of their graphical presentation such as label size, number format, background shading etc. The user may also select and interact with line plots to measure quantities or attach various annotations to data series within the chart. Most of these operations are accessed via a context menu that appears when the user right clicks the mouse anywhere within the chart window. Alternatively measurement tools may be selected from the main menu or main toolbar

In general, interacting with charts and data series fall into three main categories:

**Customizing chart visuals** involves right clicking anywhere on the chart background and changing visual attributes such as access to logarithmic scale, background color, numerical accuracy of legends and axis labels etc.

**Measuring data sets** this involves selecting a measuring tool from main menu and dragging the mouse across the chart. Measured values are dynamically extracted from the data series and displayed in a pop up window as the mouse is dragged across the chart. Measurements can be restricted to a subset of the data series by pre-selecting the desired data series before applying the measurement tool.

**Annotating data series** involves selecting one or more data sets from the chart and right clicking anywhere on the chart background and selecting an annotation to be applied to the chart data set. Usually annotations operate in toggle mode, in that, re-applying an annotation to a chart series will remove the existing annotation.

## Mouse Interaction Modes

Three icons on the main toolbar control how the mouse interacts with the chart. Mouse interaction with a chart can be in one (or none) of the following modes: selection, measure, or zoom.

**Select Chart Datasets,**  **,** enables the selection of one or more data sets in the chart window. Selected datasets are highlighted and subsequent dataset operations are applied to all selected datasets. Generally, if no datasets are selected then dataset operations are applied to **ALL** displayed datasets.

**Measure,**  **,** interactively measure and display raw dataset values or computed quantities derived from the dataset directly on the chart.

**Zoom,**  **,** zooms into regions of chart data sets adjusting the axes as appropriate. Clicking the left mouse button when the mouse is over the chart and dragging the mouse from the top left hand corner towards the bottom right hand corner will select a region highlighted in blue which represents the zoomed region. To un-zoom a chart, hold the left mouse button and drag the mouse from the bottom right hand corner towards the top left.

## Selecting Line series

Left-clicking the mouse on a displayed line series will select that line series. Multiple line series may be simultaneously selected within a chart. A selected series is indicated by overlaying square symbols on top of the line plot. Measurement interactions usually apply to all line series on the chart, but maybe restricted if one or more line series are specifically selected. Annotation interactions usually require that at least one line series be selected.

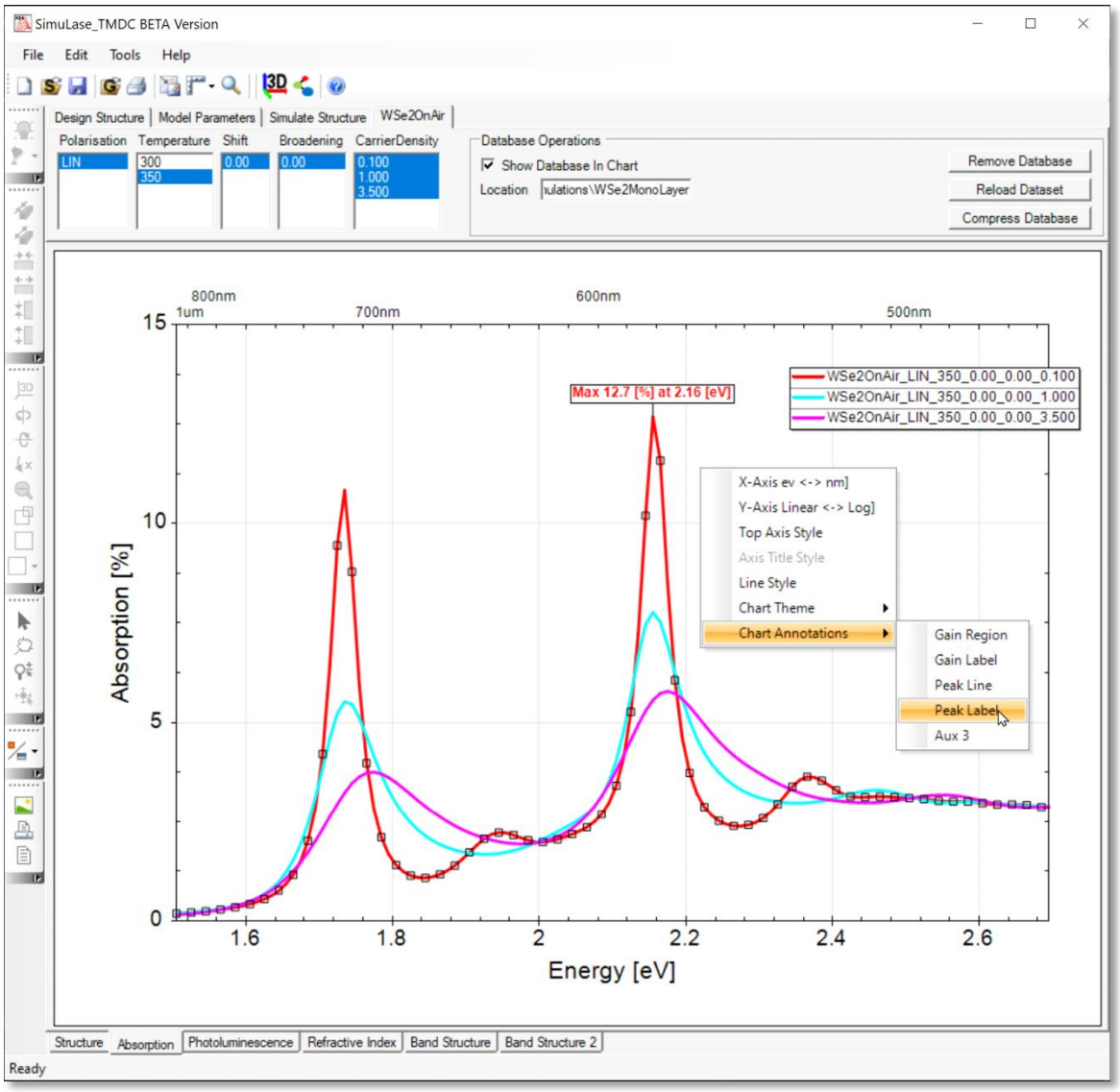



Figure 15 Selecting datasets within a chart

## Chart Context Menu

Various operations may be applied to the whole chart or to one or more line series by right-clicking the mouse anywhere on the chart.

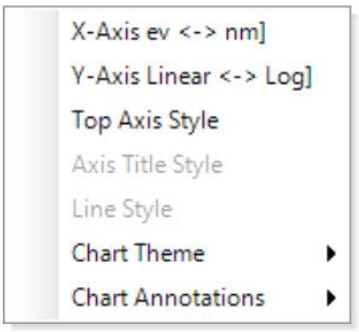



Figure 16 The main chart context menu

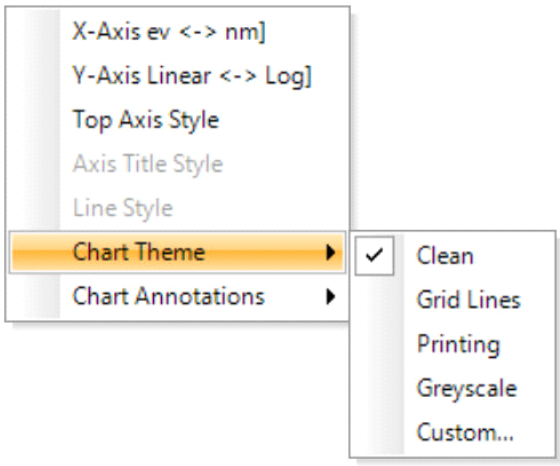
**X-Axis eV <-> nm** This will toggle the units on X axis from Energy in electron Volts to Wavelength in nanometers. The secondary X axis on top of the chart will toggle accordingly.

**Y-Axis Linear <-> Log** This will toggle the Y axis from a linear scale to a logarithmic scale

**Line Style** This opens a dialog that allows to change drawing style, color and line thickness of the selected data series.

## Chart Themes

Chart themes enable the user to quickly change the appearance of a chart in order to make your data presentation look exactly the way you like. SimuLase_TMDC provides 4 predefined chart themes and also allows the user access to fully customize all graphical attributes of the chart.




**Clean** This provides an uncluttered presentation suitable for on screen viewing and analysis of datasets. This is the default setting when SimuLase is started.

**Grid Lines** In addition to the major gridlines, this theme adds dotted horizontal and vertical gridlines at the minor axis scale tick marks.

**Printing** This provides a chart presentation suitable for publishing or screen presentation where the chart size is reduced. It improves chart legibility by increasing the font size on all axes titles and axis scales relative to the chart area and reducing the number of major tick marks and the number of decimal places in tick labels.

**Custom...** SimuLase_TMDC makes it easy to create custom user interface themes based on any of the existing ones. Selecting this option will cause a property control to appear as shown below.

## Custom Chart Themes

Selecting the **Custom...** option from the Chart Theme context menu will display the Chart Theme property Grid as shown

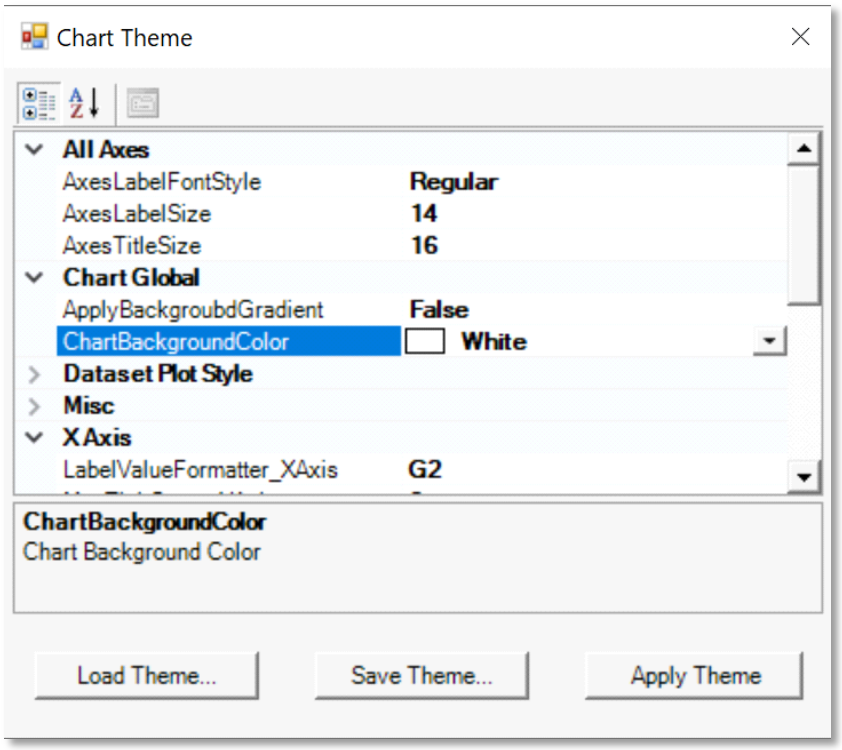



Figure 17 The Chart Theme Property Grid

The Chart Theme Property Grid control displays all the user customizable properties of a chart in a user-friendly way, enabling end users to edit the visual properties as desired to construct a custom chart. Properties are organized into named categories that group related properties according to their function. At the top is the toolbar, which allows the properties to be classified by category or listed alphabetically by property name. The central window lists properties in a <name-value> format. At the bottom is a help text that provides a brief description of the property that the user has selected.

Most basic types of properties are simple text that the user may edit directly to change the value of type of the displayed string or numeric value in general.

More complex entries provide sophisticated default editors for value types or select from a list of predefined available values. For example, a property of type Color has a drop-down list that lets you select any available color as shown.

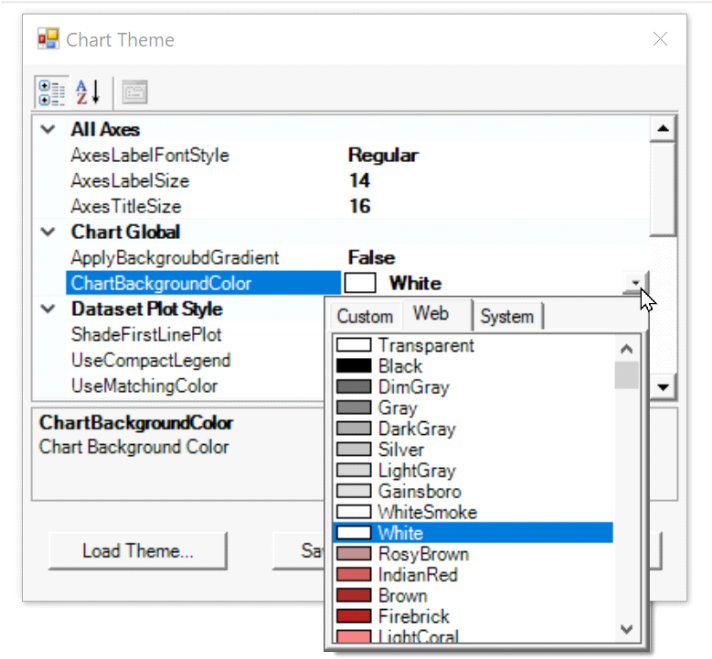
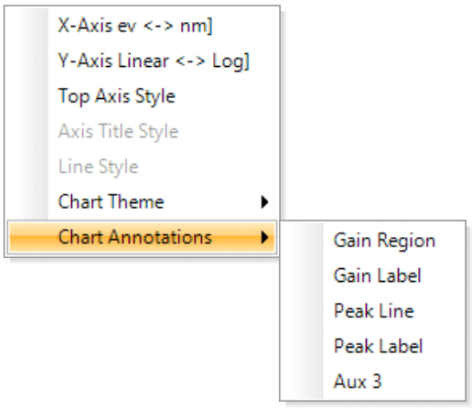



Figure 18 The color selector drop-down in the Chart Theme Property Grid

## Chart Annotations

Selecting the Chart Annotations on the context menu allows the user to attach annotations that highlight certain aspects, for example the location and peak value of a data set, or the gain region on an Absorption chart.



**Gain Region** highlights the region over which the absorption exhibits gain by using a band of transparent color that matches the color of select data series line plot. Multiple overlapping gain regions may be drawn on the chart.

**Gain Label** highlights the region over which the absorption exhibits gain (negative absorption) – if such a region exists - by adding an additional label to the X axis scale. Multiple overlapping Gain Labels may be added to the chart axes.

**Peak Line** finds the maximum numeric value in the data set that has been selected using the Select Chart Dataset, , option and inserts a color matching vertical marker line and text detailing the X axis location and numeric value of the peak.

**Peak Label** finds the maximum numeric value in the data set that has been selected using the Select Chart Dataset, , option and inserts a color matching text box above the peak detailing the X axis location and numeric value of the peak.

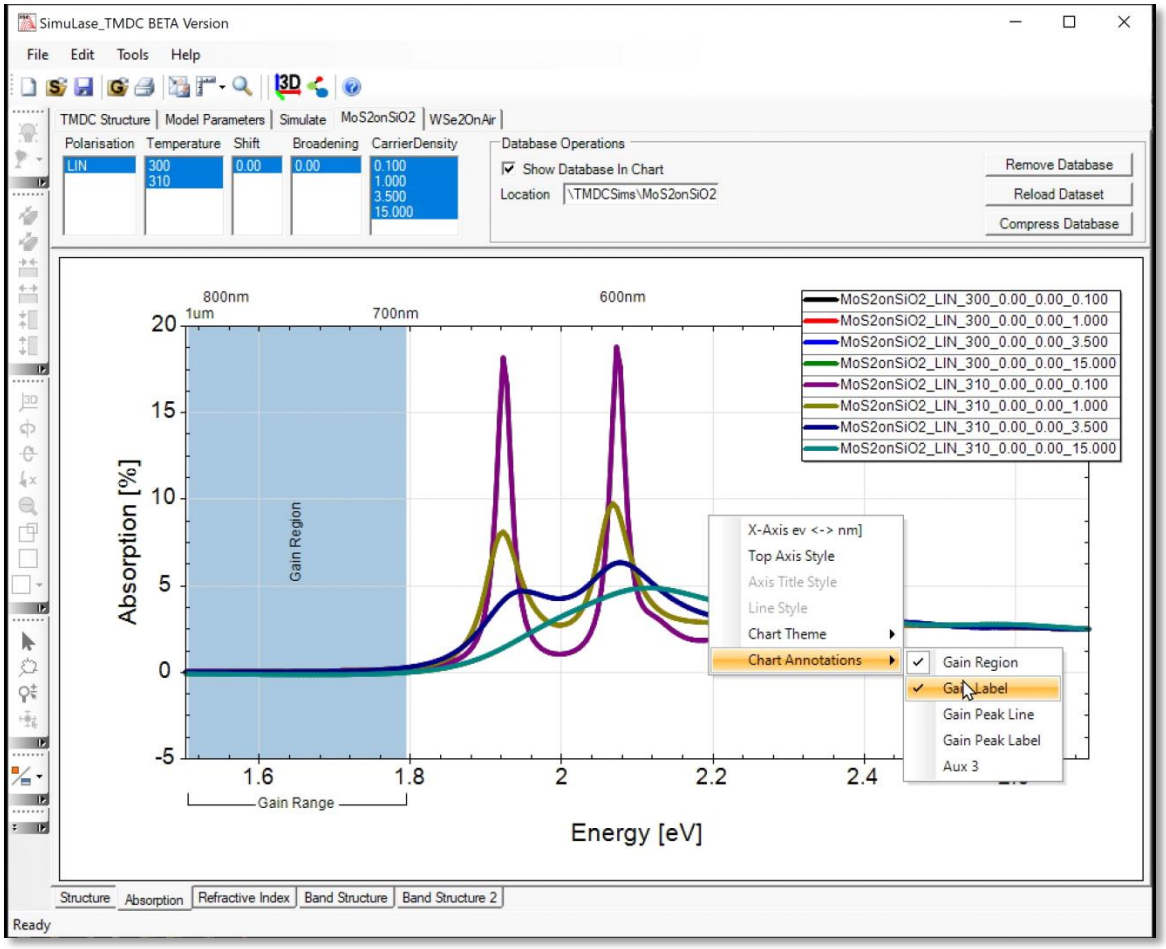



Figure 19 Chart showing both Gain Region and Gain Label annotations

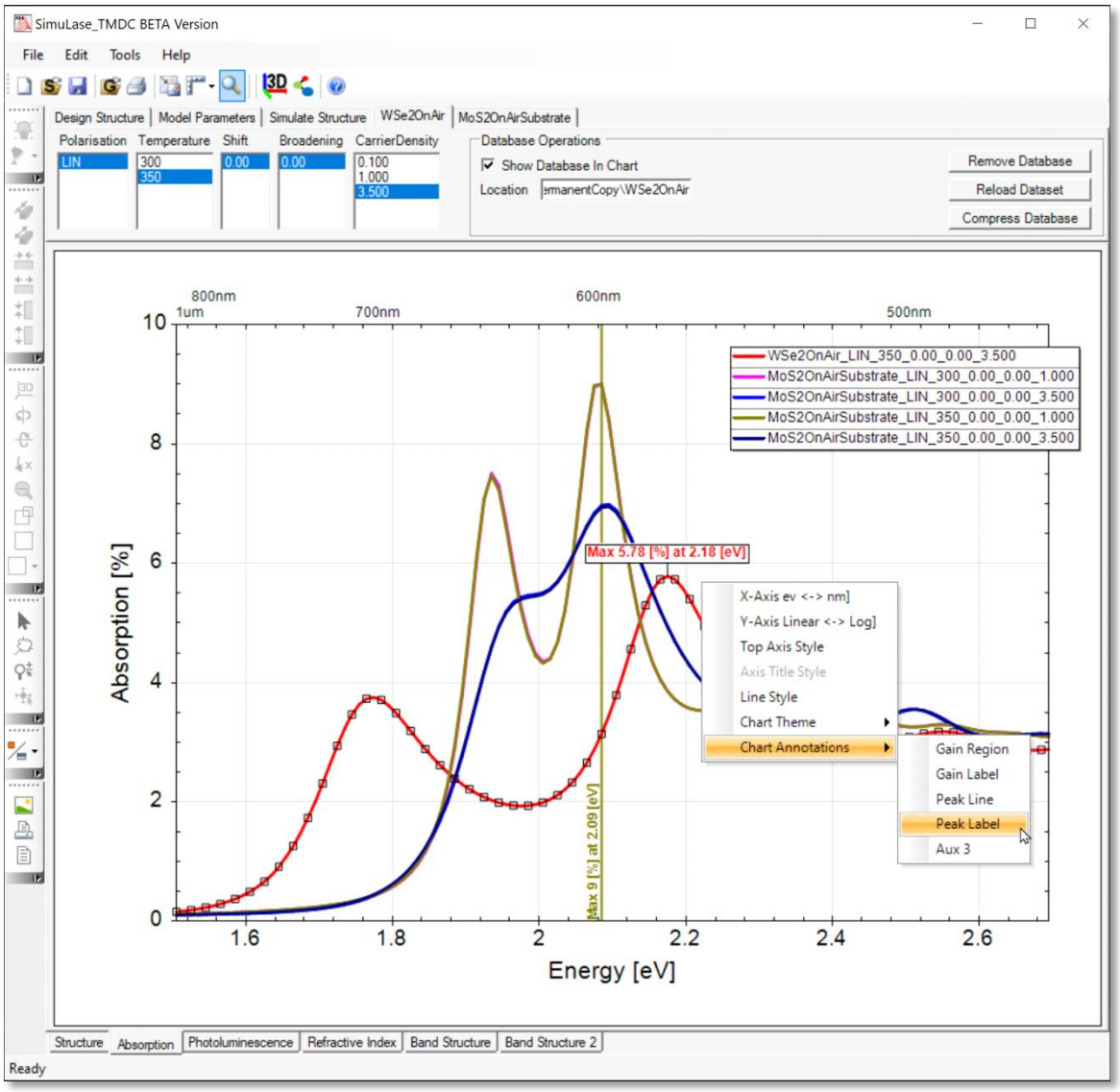



Figure 20 Chart showing both Peak Line and Peak Label annotations.

## Measure Dataset Value

In addition to attaching visual annotations to data series it is also possible to interactively measure and display a subset of raw or derived quantities from the loaded dataset. The measurement results displayed depend on the selected tool and the type of data contained in the chart.

The Measure Dataset Value tool is activated by selecting from the main tool bar and clicking into the graph. This will change the mouse pointer to a crosshair cursor that displays the exact X-value and a list of Y-values read from each of the selected data series. If no data series is currently selected, then the values are presented from all displayed data series.

The following image shows the Measure Dataset Value tool as used in an Absorption chart. The floating panel shows the current Energy value in the header and a list of Absorption values for all displayed data series. If a data series exhibits gain (negative absorption) then that value is highlighted in yellow.

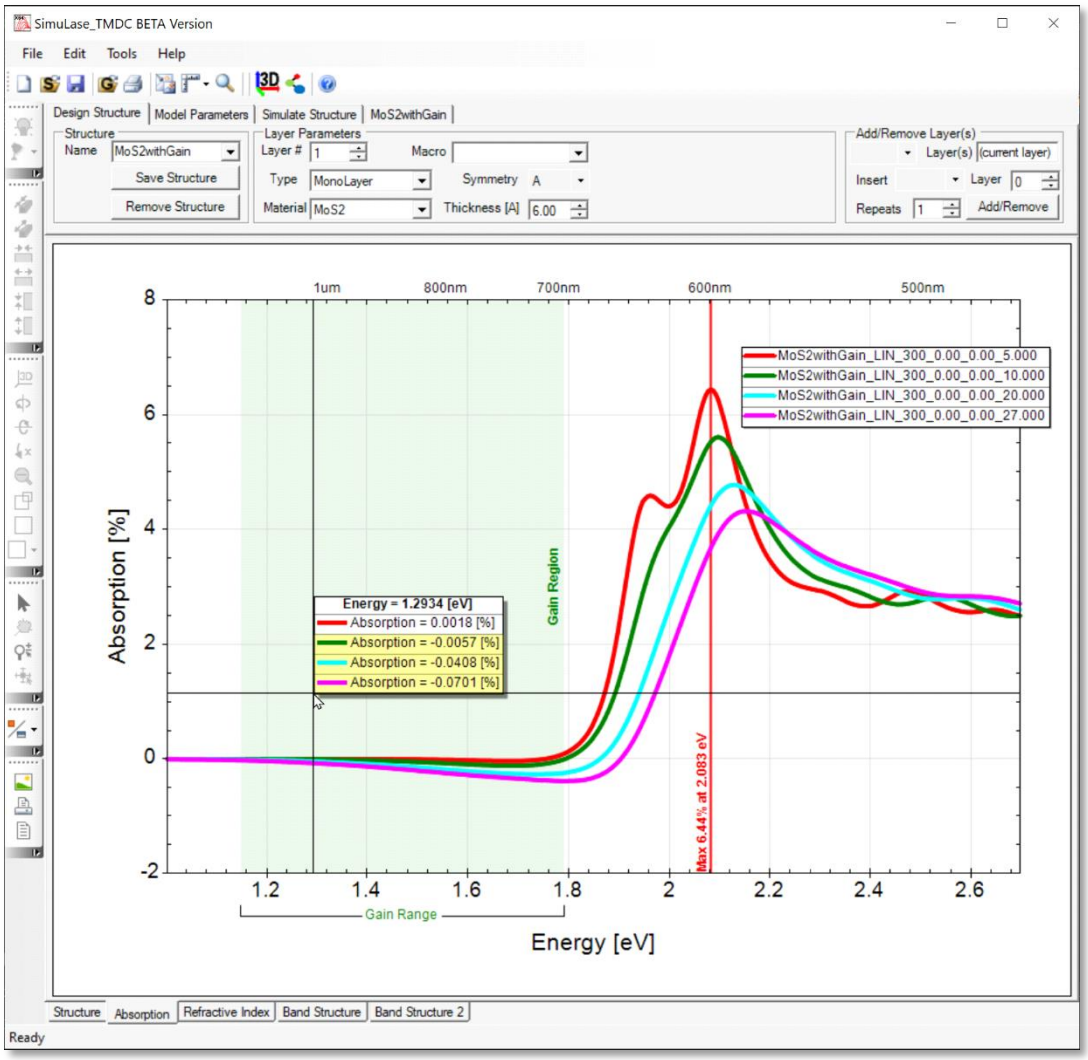



Figure 21 The Measure Dataset Value tool in an Absorption chart

## Band Structure Chart

The Band Structure chart displays the density and temperature dependent conduction ad valence bands.

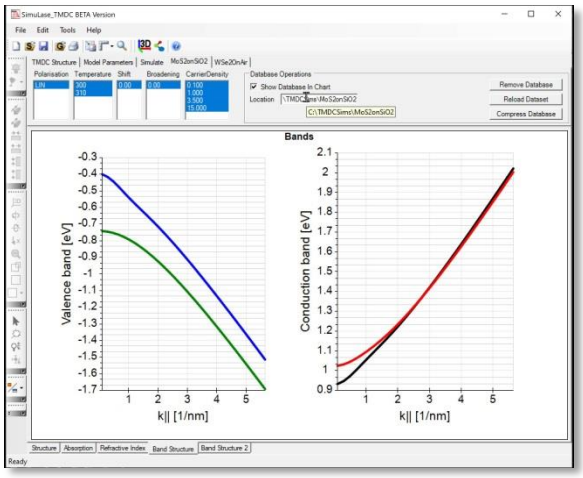



Figure 24 Band Structure chart

## Band Structure 2

The Bands Structure 2 chart displays the bands of a database in an alternative form to that of the Band Structure chart.

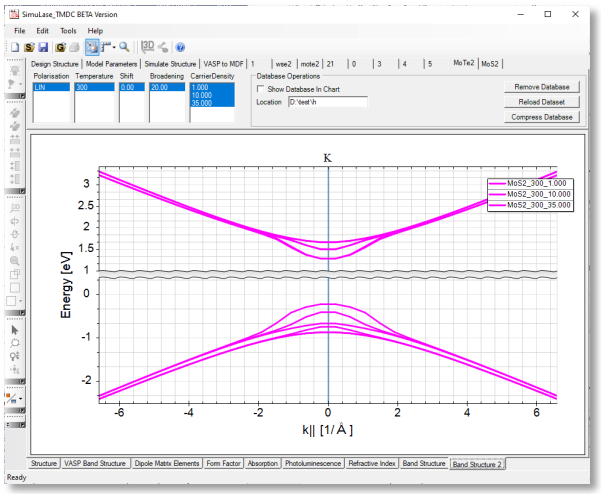



Figure 22 Bands Structure 2 chart

# General Analysis tools

Analysis tools, accessible via the tab **'Tools'** of the main menu, generally operate on the loaded datasets and produce derived quantities usually independent of the device geometry. Activating any tool will add a new tab to the **Control Group Tabs**, containing all the controls used to interact with the tool, and one or more new chart tabs to the **Data Chart Tabs** to plot the derived quantities.

## VASP_to_MDF Tool

The VASP_to_MDF tool allows to determine essential material parameters required for a simulation within the MDF model from the output of a VASP DFT calculation. Once these parameters are combined with some additional parameters as described in main manual, the data can be used to describe a user defined TMDC material using the Material Type *DFT_MDF*.

Selecting the VASP_to_MDF tool from the Tools menu adds the control tab shown in Fig. 26 to the Control Groups Tab. The controls on this tab are used to:

1) Locate a pre-existing folder containing the output from a VASP simulation.

2) Identify a destination folder and name for the file into which to save the derived MDF model parameters.

3) Present a set of numeric controls that enable the user to modify the MDF fit parameters if the user is not fully satisfied with the auto generated fits.

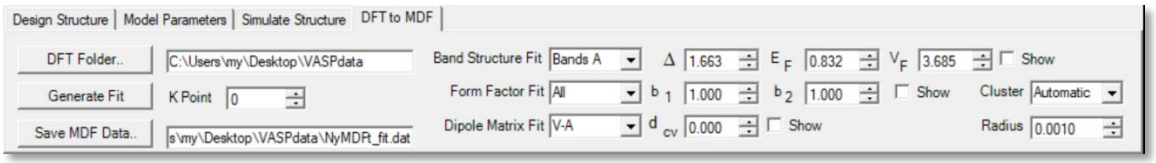



Figure 23 The VASP to MDF Controls

**DFT Folder** selects the location of the DFT (i.e.VASP) data files on disk. At a minimum the folder must contain the WAVECAR file. By default, the automatically determined values for the MDF parameters are written to a file named *Default_fit.dat* in the VASP folder as specified here.

**K Point** selects the index of the VASP output momentum grid point that is the K-point of the Brillouin zone. The index '0' indicates the first k-point contained in the VASP output.

**Generate Fit** starts the determination of the MDF parameters.

**Save MDF Data** selects the location where the generated MDF parameters will be placed. The MDF name is initially assigned the name ***Default*** but should be changed by the user when generating a new MDF material. The parameters are written to the file *name_fit.dat* where '*name*' is the name as specified here.

Once a VASP Folder and K-Point have been specified, Generate Fit will initialize the extraction of the electron and hole A- and B-bands from the WAVECAR file and calculate the dipole matrix elements and Coulomb form factors using the wavefunctions as saved in the WAVECAR file. Details of this analysis can be found in the full manual.

Once the evaluation of the VASP data has completed, three new tabs are added to the Data Chart Tabs along the bottom of the graphics window. These tabs display **VASP Band Structure**, **Dipole**

**Matrix Elements** and **Form Factor** plots. The user may overlay plots showing fits to the data according to the MDF model.

In the example shown below the VASP calculation was done for a grid that contained three lines. One going from $K$ halfway to $\Gamma$. One going from $K$ halfway to $K'$ . And, one going from $K$ halfway to $\Lambda$.

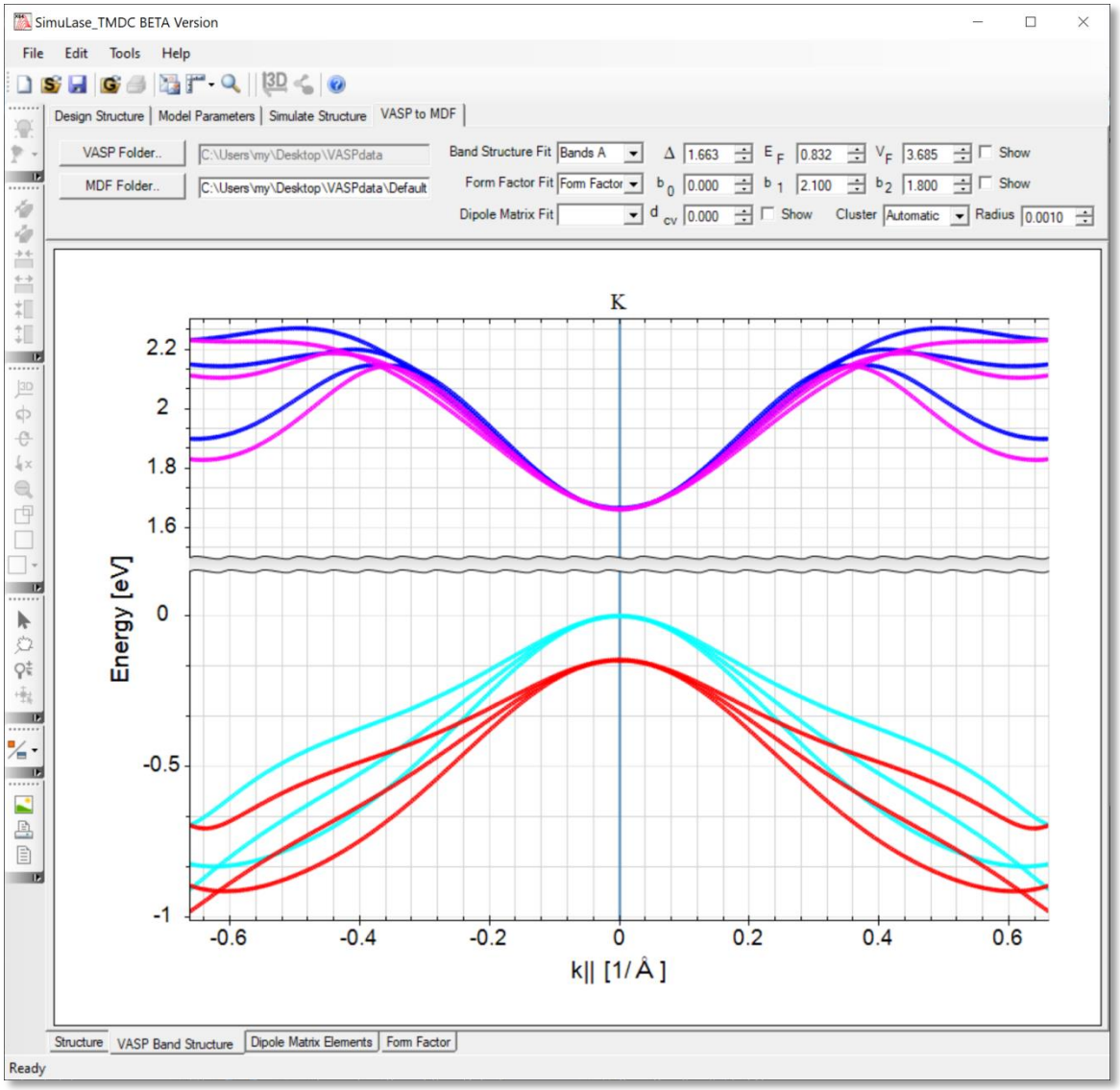



Figure 24 Band structure data imported directly from the VASP

**VASP Band Structure** tab displays the band structure plots of the electron and hole A- and B-bands as determined from the VASP output. Additionally, plot showing the auto generated fits to the various conduction and valence bands may be overlaid on the chart. Changing any of the fit parameters will dynamically update the associated fit plot in the chart.

**Dipole Matrix Elements** tab displays plots of the dipole matrix elements between the A electron and hole band and between the B electron and hole band. The associated MDF fits to that data can be overlaid.

**Form Factor** tab displays plots of the Coulomb form factors and optionally the associated MDF fits to that data.

Form factors are calculated and displayed for interband transitions, *_mat_ns_cv.dat, as well as for conduction and valence band intra-band transitions, *_mat_ns_cc.dat, *_mat_ns_vv.dat. As described in the main manual, within the model implemented in SimuLase_TMDC the form factor is assumed to be directionally independent and given by an average over inter- and intraband form factors. The fit to the data should try to find an average with respect to the band association and directional dependence.

The rest of controls on the **VASP to MDF** tab enable the user to dynamically view and modify the MDF parameters fits to the VASP data and how the data is displayed on the chart.

**Band Structure Fit** This line of controls enables the user to select the A or B bands and to modify the fit parameters for the bandgaps $\Delta$, for the Fermi energies, $E_F$, and for the Fermi velocities, $v_F$. The **Show** check box is used to show or hide the associated fit curve overlaid on the chart.

**Form Factor Fit** This line of controls enables the use to select either the Form factor and modify the fit parameters $b_1$ and $b_2$. The Show check box is used to Show or Hide the associated fit curve overlaid on the chart

**Dipole Matrix Fit** This line of controls enables the use to select either Band A or Band B and modify the fit of the dipole matrix element $d_{cv}$.As outlined in the main manual, the dipole matrix element is the one at the K-point. The directional and momentum dependence of the dipole matrix elements is taken into account analytically within the MDF model. Thus, the fit shown here is just a line at the momentum independent value of the matrix element at K. The **Show** check box is used to show or hide the associated fit line on the chart.

In each of the VASP to MDF charts, visual representation of the Band Structure, Dipole Matrix Elements and Form Factor curves may be modified by using the **Cluster** and **Radius** controls. The controls dictate the density of points used to represent the raw data. Reducing the point density highlights the overlaid solid line fit curves.

**Cluster** determines how many datapoints of the calculated data are displayed in the graphs. This control can be used to reduce the amount of displayed data points in order to be able to see more clearly the fit-lines amongst the symbols representing the VASP data. The clustering mode can be set to three possible modes:

*Automatic* attempt to render the dataset as a smooth continuous curve without over plotting unnecessary data point.

*Enabled* allows the user to manually set a density of points used to represent the data set.

*Disabled* displays a single dot symbol on the chart for every data point in the original.

**Radius** sets an exclusion radius around the displayed data points. Increasing the radius value reduces the level of detail with which the raw data is plotted. Lower radius values will result in more accurate representation of the data set, at the cost of more points being plotted

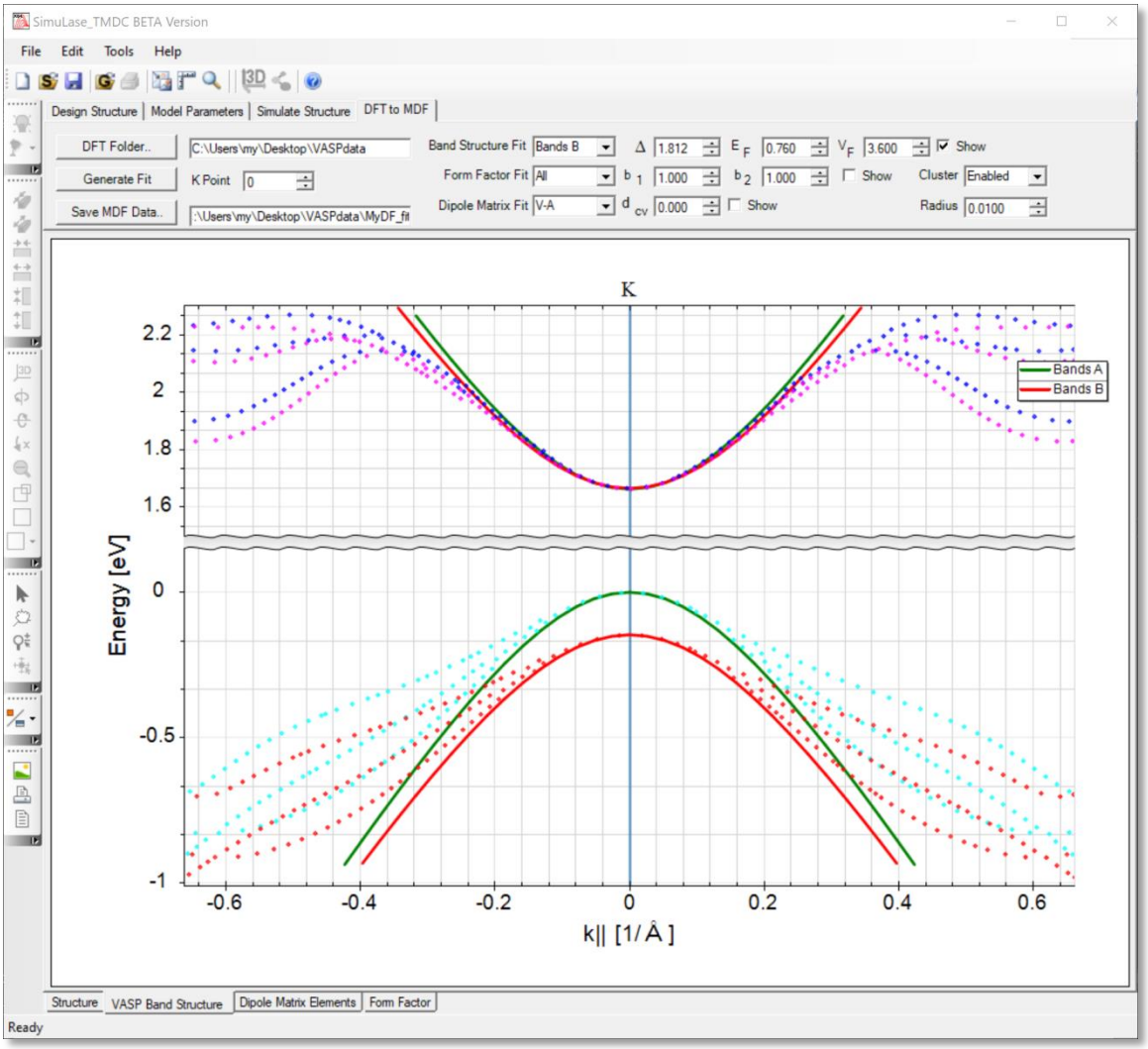



Figure 25 VASP Band Structure plots with overlaid MDF bands

## 3D Structure Visualization

SimuLase_TMDC possesses the capability to render layered structures as 3D objects with full control over visual aspects such as camera orientation and lighting. The primary use of these 3D capabilities is to produce 3D renderings of TMDC based structures for presentation purposes. The 3D visualizations of the structure have no influence on the numerical simulation of the structures and should be considered a graphical rendering tool only.

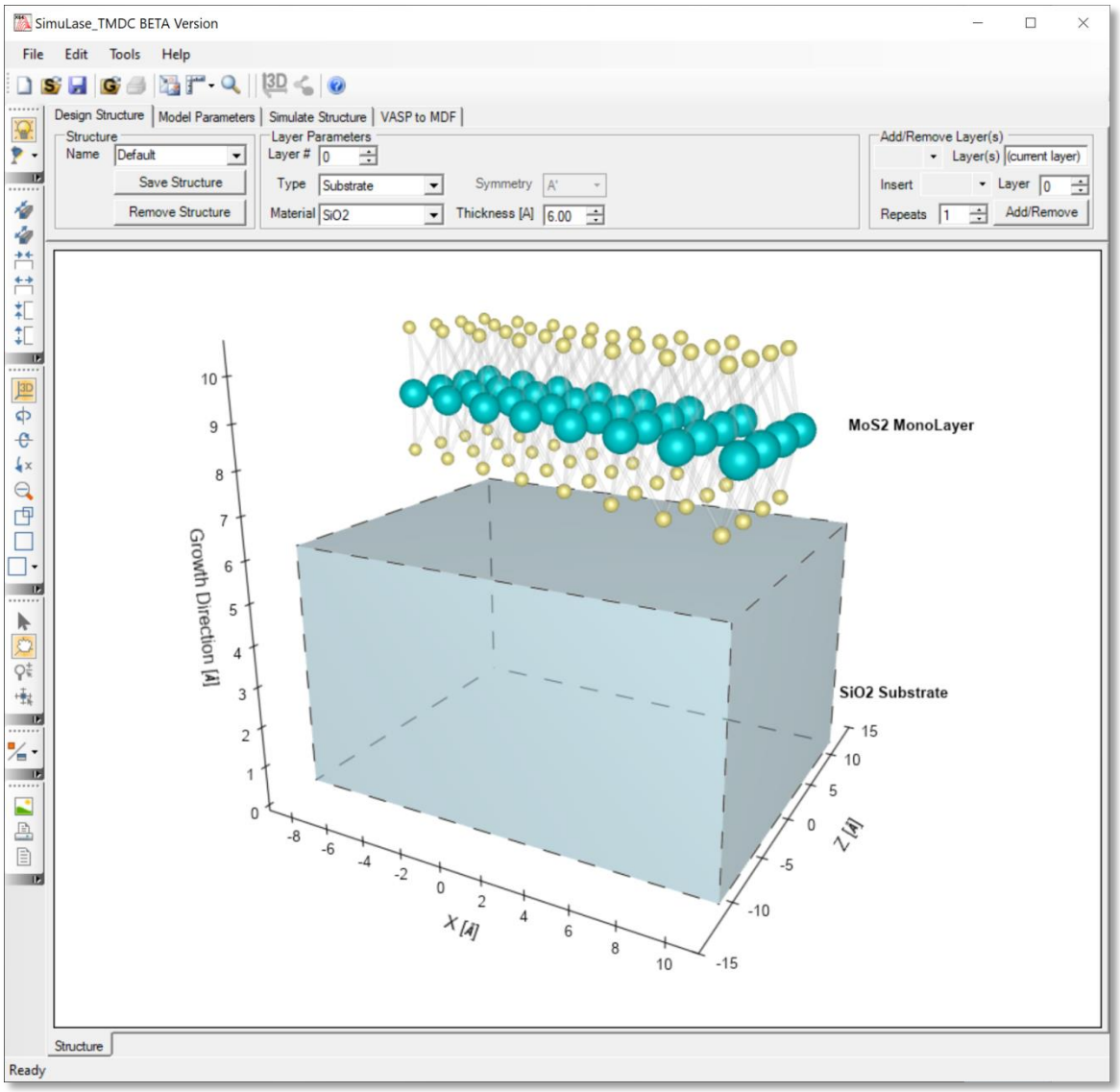



Figure 26 The layered device structure rendered as 3D object.

Most of the controls related to the 3D aspects of a structure rendering appear as icons in a vertical toolbar on the left hand side of the main window. Hovering the mouse pointer over an icon will pop-up a tool tip describing the action the icon will perform.

By default SimuLase_TMDC renders structures in 2D with false shading applied to the ball and stick renderings of TMDC molecules giving them a spherical appearance. A flat unshaded 2D view of the structure is also available and is always applied when outputting graphics to PDF file format.

## Activating Full 3D Visualization Mode

To activate full 3D Mode, click on the on the "Trackball" icon, on the vertical tool bar at the left hand side of the screen, and then drag the mouse anywhere on the 2D structure, causing the 2D

rendering to rotate into the third dimension. This simultaneously enables all the 3D manipulation control icons on the vertical toolbar.

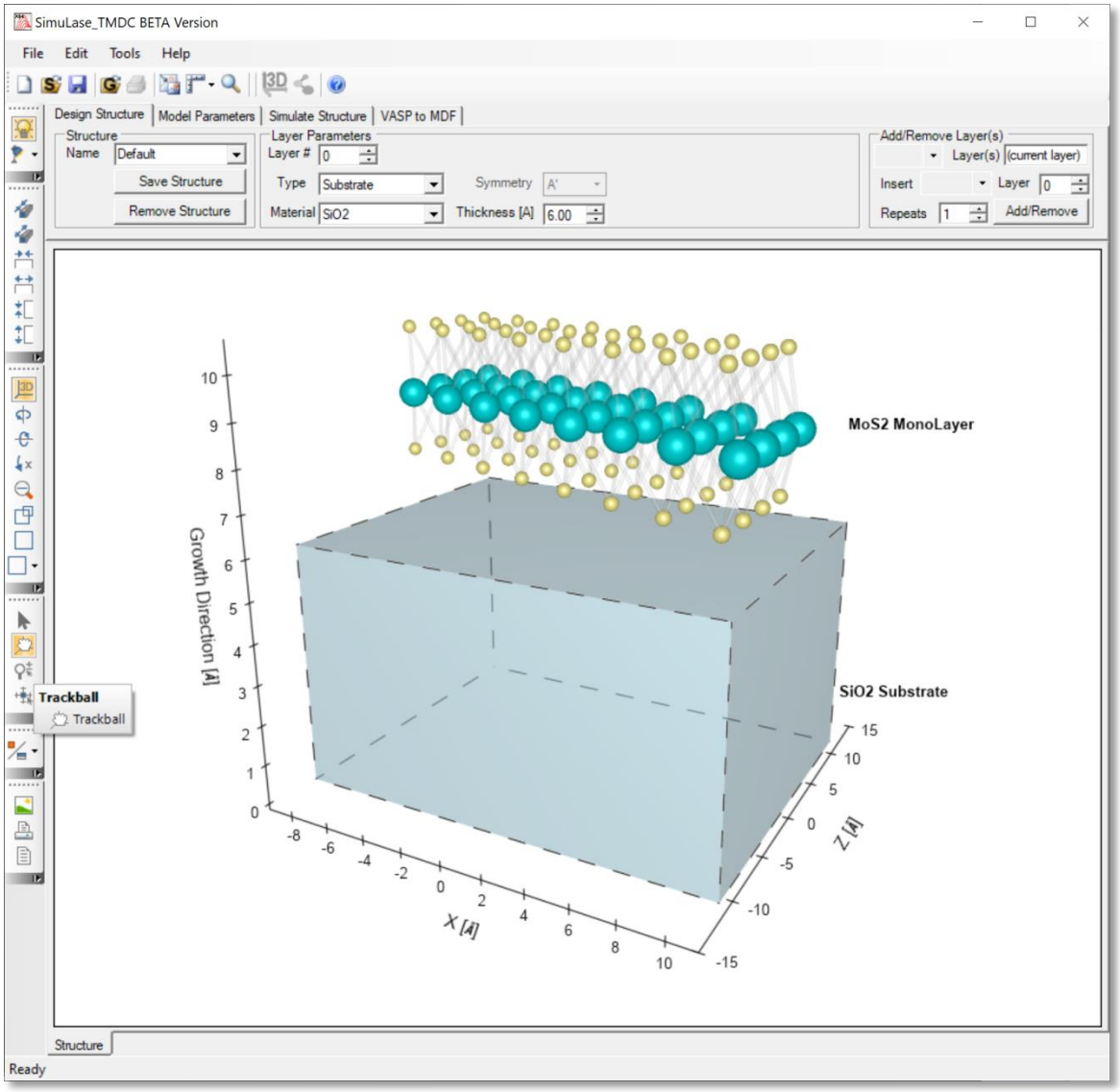



Figure 27 Rotating the structure into the third dimension using the Trackball tool.

To produce a visually more convincing 3D rendering of the structure the user should enable the “Perspective Projection” icon in the vertical 3D toolbar.

## 3D Structure rendering controls

A brief description of each of the 3D control icons is given below. The most frequently used controls controls are expanded on in the following sections. Controls are grouped according to the operations they perform on the 3D rendering of the structure.

### *Lighting Controls*

**Toggle Lighting**: Turns and off the virtual light sources illuminating the model
**Toggle Lighting**: Turns and off the virtual light sources illuminating the model

### *Chart Export and Printing Controls for 3D structures*

**Export Chart Image**: Export the current chart to file as a raster, (BMP, PNG, JPEG etc.) or vector (SVG) image.
**Print**: Opens the built-in print manager dialog
**Page Setup**: Configure size and orientation of the page layout before printing

### *Structure Aspect Ratio Controls*

**Decrease Chart Depth**: Decreases the 3D depth of the structure rendering
**Increase Chart Depth** : Increases the 3D depth of the structure rendering
**Decrease Chart Width**: Decreases the 3D width of the structure rendering
**Increase Chart Width**: Increases the 3D width of the structure rendering
**Decrease Chart Height**: Decreases the 3D height of the structure rendering
**Increase Chart Height**: Increases the 3D height of the structure rendering

### *Hardware Rendering Controls*

**Render Surface**: Selects if rendering is done on CPU (bitmap) or employs GPU acceleration (window)

Render Surface determines the hardware (CPU or GPU) used to render the 3D image on the screen. The default render surface in SimuLase_TMDC is set to **Bitmap**, in this mode the chart will NOT leverage any installed GPU hardware,. An alternative render mode, **Window** is also available. When this mode is selected the entire graphics rendering is done using the GPU which results in much higher rendering speed. The **Bitmap** mode is more compatible with a broader range of hardware since it does not depend on an installed GPU and the associated drivers. The most noticeable effect of using bitmap rendering is a reduction in graphic rendering performance and responsiveness when rotating complex structure containing many lattice atoms.

### *Mouse interaction Controls for 3D structures*

**Mouse Select tool**: This tool is used to interactively select structure layers via the mouse
**Trackball tool** : This tool helps you interactively change the camera position to rotate it around the structure rendering
**Mouse Zoom tool**: This tool helps you interactively zoom in and out the structure rendering
**Mouse Offset tool**: This tool helps you interactively position the structure rendering within the main window

### *3D View and Rendering Controls*

**Toggle 3D**: Toggles between a full 3D rendering or 2D flat rendering of the structure
**Rotate Right**: Rotate structure rendering around the Y-Axis
**Elevation Up**: Rotate structure rendering around the X-Axis
**Viewer Rotation Right**: Rotate structure rendering around the X-Axis
**Zoom Out**: Zoom out of the viewer, decreases the apparent size of the structure rendering
**Perspective Projection**: Enables the perspective projection view of the structure rendering
**View 2D**: Enables a predefined 2D orthogonal projection of the structure onto the screen maintaining the 3D shading.
**Predefined Projection**: List of predefined viewing directions of the structure at various angles and rotations

## Exporting Chart Images and Printing

From the main menu bar the user may select **File | Save Chart As Image...** to export the currently active chart or 3D visualizations of the device structure into many standard raster and vector graphic formats such as JPG, SVG, PNG and PDF, at user selectable resolutions.

From the main menu bar the user may access the Windows printer subsystem, enabling printing capabilities, such as Page Preview, Page Setup and Printer selection etc., for any SimuLase_TMDC chart or 3D rendering of a device structure.