



## Supporting Information

### The Next Dimension of Structural Science Communication: Simple 3D Printing Directly from a Crystal Structure

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**This document includes:**

Guidance on Cleaning a 3D Model File

## Guidance on Cleaning a 3D Model File

### Why do I need to do this?

If you are intending to use one of the popular web-based services like [Shapeways](#), [Sculpteo](#) and [i.materialise](#), then you simply don't need to worry about cleaning up the 3D model file. These services already have excellent software and automated processes to clean up your model and there won't be any issues. A lot of the newer, more expensive, 3D printers available to buy also come with sophisticated software to clean your computer-designed 3D model.

If, however, you are not using a web-based service, then you may occasionally experience an issue during printing due to the way that the 3D model is built. Mercury represents atoms and bonds within the 3D model as a collection of intersecting hollow mesh spheres and cylinders, rather than as a single solid object. In some cases, this can result in disconnects or gaps between parts of the model when they are 3D printed.

The easiest way to address this possibility prior to 3D printing is to use an additional post-processing step to "clean up" the 3D model and ensure safe 3D printing. There is a wide range of software tools that can help you to check and clean your 3D model.

### Recommended software options

The Windows application, 3D Builder, is an excellent option if you are using either Windows 8 or 10. You can load your VRML or STL model file into 3D Builder and use the Smooth and Simplify options to clean the model file. The 3D Builder application will also allow you to easily optimise the orientation of your molecule for easy 3D printing using the Object > Settle option. This will find the flattest orientation for the model to increase strength and reduce both print time and the amount of support material needed.

Autodesk's application, [MeshMixer](#), only accepts STL files and not VRML files, but this has a very effective option under Edit > Make Solid, which generates a solid model file from the collection of intersecting meshes. MeshMixer also has a range of quality settings for this solidification method ranging from "Blocky" to "Sharp Edge Preserve".

Alternative programs such as [Netfabb](#), [MeshLab](#) and [Magics](#) also have a range of options to clean up your 3D model file and realign for more effective 3D printing.