

**A Matlab script (`surf_print.m`) to create 3D-printable objects from 2D functions (surface plots) by  
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The code `surf_print.m` is a Matlab script that converts 2D surface-plot data into 3D models (STL files). We have used this to make models of molecular potential energy surfaces, but the script could be applied to other types of data sets. The code runs successfully with Matlab versions 2012b and 2013a and should also work on older versions. The code comes with an excel file – `test.xlsx`. It needs to be located in the same folder as the Matlab script. It contains three sheets – Xdata, Ydata and Zdata for the X, Y and Z data respectively. Xdata and Ydata each consist of a vector of the grid points for that coordinate and Zdata consists of the corresponding surface data matrix. The script imports all of the data from Excel to Matlab, so it is recommended to only include the required data in the Excel file. Simply replace the example data with your data to generate a 3D model. The data in the example file describes the lowest singlet surface of CO+O in a 200x200 array (the script will automatically accommodate other array dimensions). The number of columns of Zdata should match the number of X-grid points, while the number of rows of Zdata should match the number of Y-grid points.

The coordinate ranges (for approach of O(<sup>1</sup>D)-atom to a CO fragment) in the example file are as follows:

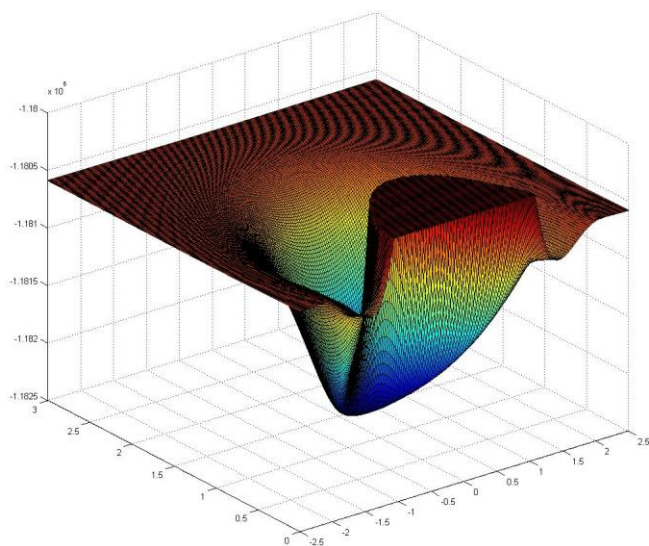
X: -2.5 to 2.5 angstroms, size - 200

Y: 0 to 3 angstroms, size - 200

Z:  $f(X,Y)$ , size - 200x200

Running the code

Once you run the script, if the data import is successful, a Matlab figure of the surface should be produced, as shown here.



The Matlab command window should then display the following text:

*"STL files don't have units.*

*We set the units in the printer.*

*For convenience let us work in inches.*

*The CO+O singlet example PES in this sheet is: 5" x 3" x 4"*

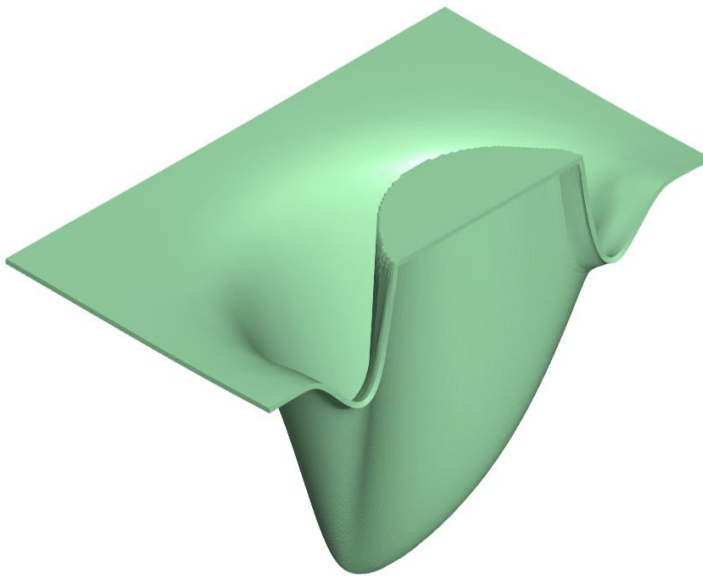
*It is important to assign proper dimensions to the object otherwise the result is a stretched/distorted final object."*

The script will then prompt you for the X, Y and Z object dimensions.

After entering the desired dimensions of the 3D object (for the example 5" x 3" x 4"), you get an option to create a mesh or not. Creating a mesh can save on material costs but it takes a lot longer to process the files in Matlab and can cause problems for the printer/object if the mesh is too fine. Creating a smooth surface, on the other hand, doesn't take much time. Note: currently the X and Y data vectors need to be of the same length (square Zdata matrix) if one desires to automatically create a mesh.

The outputted STL file is created in the same folder with the name "thick\_surf.stl", which can be opened with any STL viewing software. [3D-Tool](#) and [STL Viewer](#) are two freeware examples. STL viewer enables one to look at the dimensions of the object, while 3D-Tool is a faster tool to view multiple objects.

The following is an image of the Singlet surface example, with the thickness specified as 0.05 inches.



For more details, contact Richard Dawes – dawesr@mst.edu.