
Subject: Re: Molecular models and contour maps
Posted by [Mark Hadfield](#) on Tue, 30 Jul 2002 05:08:09 GMT
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From: "Rick Matthews" <matthews@wfu.edu>

- > I want to use IDL for help with 3-D visualization of electron
- > density calculations. I want like IDL to display a ball and stick
- > model of a molecule, with interleaved contour maps of the density
- > surrounding the atoms in planes of my choosing.

IDL can certainly do this.

The IDL Object Graphics system is (for the most part) a collection of building blocks with which you can build visualisations. You have to assemble the building blocks yourself. This is simple in principle but there are a lot of details to learn and you will encounter a few surprises.

- > I have not found visualization routines to generate 3-d displays of
- > the balls for atoms or sticks connecting them. Is there a
- > straightforward way to do this?

Routine MESH_OBJ generates data describing a simple shape like a ball or a cylinder. You pass the data to an IDLgrPolygon object to display the shape. You then mount the IDLgrPolygons in IDLgrModel objects to translate, scale & rotate them. You can use XOBJVIEW to display the collection of IDLgrModels.

I suggest you search the group archives at <http://groups.google.co/m> for a thread earlier this month entitled "Plotting on a sphere". While you're at it, try a search for "mesh_obj".

- > If I succeed in 1, is there a way to display planar contour maps in
- > the image?

The IDLgrContour object implements planar (or non-planar) contour-map objects.

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