Subject: Re: Molecular models and contour maps
Posted by Rick Matthews on Thu, 01 Aug 2002 20:47:27 GMT
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Rick,

This is *extremely* helpful. Thank you very much.

This should get me off to a good start.

Rick

Rick Towler wrote:
> "David Fanning" <david@dfanning.com> wrote
>
>> Rick Matthews (matthews@wfu.edu) writes:
>>
>>
>>
>>> 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.
>>>
>>> 1. 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?
>>> 2. If I succeed in 1, is there a way to display planar contour
>>> maps in the image?
>>
>> Uh, Rick, our friend Rick Towler will get back to you ASAP. :-)
>
>
> Sorry to take so long ;), I am trying to get a manuscript out the door and
> my pdf maker has decided to stop working.
>
>
> For 1 you can use the oh so handy "orb" object for the balls and the
> IDLgrPolyline object for the lines. The orb is undocumented but the source
> can be found in $RSI_DIR\Files\RSI\IDL55\examples\visual which contains a
> description of the keywords and properties.
>
> Basically you create an instance like so:
>
> atom1 = obj_new('orb', pos=[0,0,0], color=[255,0,0], $
>   radius=0.5, density=1.0)
>
> since orbs are a subclass of IDLgrModel you can throw an orb right into

> xobjview:
>
> xobjview, atom1
>
>
> Now it has been a while since I used styrofoam balls and toothpicks to stick
> together my favorite molocules but here is something to start with:
>
> ; a couple of hydrogen atoms
> h1 = obj_new('orb', pos=[-2,0,0], color=[200,200,200], radius=0.5)
> h2 = obj_new('orb', pos=[0.61,2,0], color=[200,200,200], radius=0.5)
>
> ;an oxygen atom
> o = obj_new('orb', pos=[0,0,0], color=[255,0,0], radius=1.0)
>
> ; make the sticks
> x = [-2,0,.61]
> y = [0,0,2]
> z = [0,0,0]
> sticks = obj_new('IDLgrPolyline', x,y,z, color=[0,0,0], thick=20.0)
>
> ; put everything in a model
> water = obj_new('IDLgrModel')
> water -> add, [sticks, h1, h2, o]
>
> ; view the model in xobjview
> xobjview, water, /block
>
> ; clean up our objects
> obj_destroy, [sticks, h1, h2, o]
>
>
> Obviously this could get complicated but I can see the process simplified by
> creating some basic objects that include your common atoms and their sticks
> and piecing them together by passing bond angles and location (I am thinking
> of the wooden stick and ball models, I don't know how sophisticated you want
> to get).
>
>
> As for 2) you can project contours onto a plane so I *think* you could do
> what you want. It just might be more work than you had hoped. But then
> again, your program will turn out so cool it will all be worth it.
>
>
> Good luck!
>
> -Rick
>

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>

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