

## Easy Jmol Web Pages using the Jmol Export to Web Function:

a tool for creating interactive web based instructional resources and student projects with live 3-D images of molecules without writing computer code.

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This function (tool) makes it easier to use live 3-D molecular visualization as part of web based tutorials, interactive text books or student projects. Other Jmol (1) web page creators require servers or additional software.(2-4)

Jmol is used extensively on the Web (5) in both research journals (6) and for educational purposes.(7,8)<sup>1,2</sup> A small number of people with experience writing html and javascript code were producing these web pages. Now web pages with "live molecules" can be created easily using the "export to web ..." function, which I developed for Jmol versions 11.4 and more recent.(9) My students use this function and the associated tutorial (see WebWare submission) to produce web pages reporting on molecular modeling computations. I also create web based chemistry tutorials using this function; there are examples in the submitted files and more at my web site.(10)

This tool provides a dialog box in the application version of Jmol with which the user can generate web pages showing live 3-D molecules. Once the page is created the user can edit the text and add other information using the web page editor of their choice. At present there are two templates: a page with static images that convert to live molecules when the user clicks on them; and a page with a

live molecule next to a scrolling window containing text and automatically generated buttons to change the live display. Possible future enhancements include: 1) addition of optional buttons that do common things to Jmol views, such as spin the molecule or change the background color; 2) a new template for a table of Jmol applets; and 3) other requests as they are made by users.

This JCE WebWare contribution (.zip file) includes:

- A tutorial suitable for use in a class on using the "export to web..." function, including a brief introduction to using the Jmol application. Two versions are provided:
  1. A browser based html version in the "How-To" directory. Entry point is the file `Export_to_Web_Tutorial_Index_Menu.html`. It may be viewed locally or by copying the whole "How-To" directory to a web server for online access. The version on the author's web site is updated regularly.*(11)*
  2. A text and static image version of the tutorial, is provided as .pdf, .doc and .odt (open document format) files. The file names used are of the form `Export_to_Web_Tutorial_JCE_Webware.XXX`, where the "XXX" is the appropriate file extension.
- Web pages in the "Examples" directory show capabilities of the Jmol applet:
  1. `Jmol_Demo.html` : continuously runs through display variations Jmol can do.
  2. `Example_1.html` : simple student report on an *ab initio* computation of ethane geometry.

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**Notes**

1. Educators should also consider the Molecular Workbench (12), which generates tutorials in the form of java applications that can be started from a web page although they are not contained within the web page. Molecular Workbench uses Jmol for 3-D molecule visualization. (13, 14)
2. For generating simple 2-D chemical animations or having students use cartoons to develop their understanding of the microscopic nature of matter consider using the Chemsense package. (15)

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10. More examples of what can be done with the "export to web..." function can be found at the

author's web site by following the links to "Interactive molecules & Jmol stuff" at <http://www.uwosh.edu/facstaff/gutow>.

11. The most up-to-date version of the tutorial may be accessed at [http://www.uwosh.edu/faculty\\_staff/gutow/Jmol\\_Web\\_Page\\_Maker/Export\\_to\\_web\\_tutorial.shtml](http://www.uwosh.edu/faculty_staff/gutow/Jmol_Web_Page_Maker/Export_to_web_tutorial.shtml); a Spanish version maintained by Angel Herráez is available at [http://biomodel.uah.es/Jmol/exporta\\_a\\_web/](http://biomodel.uah.es/Jmol/exporta_a_web/).
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