

## 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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The open source java program Jmol<sup>1</sup> is widely used to present interactive 3-D visualizations of molecules, because of Jmol's power and ability to work well with most browser/operating system combinations. A JVM (Java Virtual Machine, version 1.4 or greater), which is installed by default on MacOS and Windows machines, is all that is necessary for Jmol to run. Jmol is used extensively on the Web in both research journals and for educational purposes.<sup>2</sup> Only a small number of scientists and educators are producing these web pages containing "live molecules", because significant experience writing html and javascript code has been necessary to do so. To expedite my production of these web pages, allow my students to easily produce web assignments, and make it possible for any scientist to create web pages containing "live molecules", I extended the Jmol application by writing the "export to web ..." function,<sup>3</sup> which is part of Jmol version 11.4 or more recent.

This "export to web..." function provides a dialog box in the application version of Jmol with which the user can generate web pages containing Jmol applets. These web pages can also contain buttons that switch between the various views. Once the page is created the user can edit the text and add other information using the web page editor of their choice. Thus anyone familiar with word processing applications can create interactive molecular visualizations after learning a little about using the Jmol application. Since students do not need to be taught any web programming skills to create pages, students and instructors can concentrate on the understanding of the chemistry presented in student web projects. Chemical educators, with little or no programming experience, can now more easily use live 3-D molecular visualization as part of web based tutorials, interactive text books or student projects.<sup>4</sup>

This JCE WebWare contribution includes:

- A tutorial on using the "export to web..." function which includes a brief introduction to using the Jmol application. This tutorial is suitable for use in a class or for self instruction and is how I teach students to produce web pages to present the results of a computational chemistry project. There are two versions of this tutorial provided here:
  1. a browser based html version in the "How-To" directory. Entry point is the file Export\_to\_Web\_Tutorial\_Index\_Menu.html. You may either view it locally or copy the "How-To" directory to a web server to provide online access. A continuously updated version is maintained at my web site ([http://www.uwosh.edu/faculty\\_staff/gutow](http://www.uwosh.edu/faculty_staff/gutow)). Follow the links to "Tools for authoring Jmol web pages".
  2. a text and static image version of the tutorial, is also 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.
- Example web pages in the "Examples" directory showing some capabilities of the Jmol applet:
  1. Jmol\_Demo.html : continuously runs through some of the display variation Jmol can do.
  2. Example\_1.html : a version of the kind of thing that students can do. This page presents a very simple report of the results from an *ab initio* computation of ethane geometry.

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1. Get the latest version from: <http://www.jmol.org>
2. Web sites using Jmol ([http://wiki.jmol.org:81/index.php/Websites\\_Using\\_Jmol](http://wiki.jmol.org:81/index.php/Websites_Using_Jmol)); Journals using Jmol ([http://wiki.jmol.org:81/index.php/Journals\\_Using\\_Jmol](http://wiki.jmol.org:81/index.php/Journals_Using_Jmol)); Articles about Jmol usage: Angel Herráez, "Biomolecules in the computer: Jmol to the rescue." *Biochemistry and Molecular Biology Education* 34(4): 255-261 (2006); M.E. Cass, H.S. Rzepa, D.R. Rzepa, and C.K. Williams, "The use of the free, open-source program Jmol to generate an interactive web site to teach molecular symmetry." *Journal of Chemical Education* 82(11):1736-1740 (2005).
3. For those interested in the source, the source code and ancillaries of the webexport package can be accessed at: <http://jmol.svn.sourceforge.net/viewvc/jmol/trunk/Jmol/src/org/openscience/jmol/app/webexport/>
4. Another application educators should consider is the Molecular Workbench, 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 rendering of molecules. Xie and R. Tinker, "Molecular Dynamics Simulations of Chemical Reactions for Use in Education", *Journal of Chemical Education*, 83, 77-83 (2006); A. Pallant and R. Tinker, "Reasoning with Atomic-Scale Molecular Dynamic Models", *Journal of Science Education and Technology*, 13, 51-66 (2004) ; 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. <http://mw.concord.org>; Chemsense software and more information available at <http://chemsense.org/>.