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May, 2011

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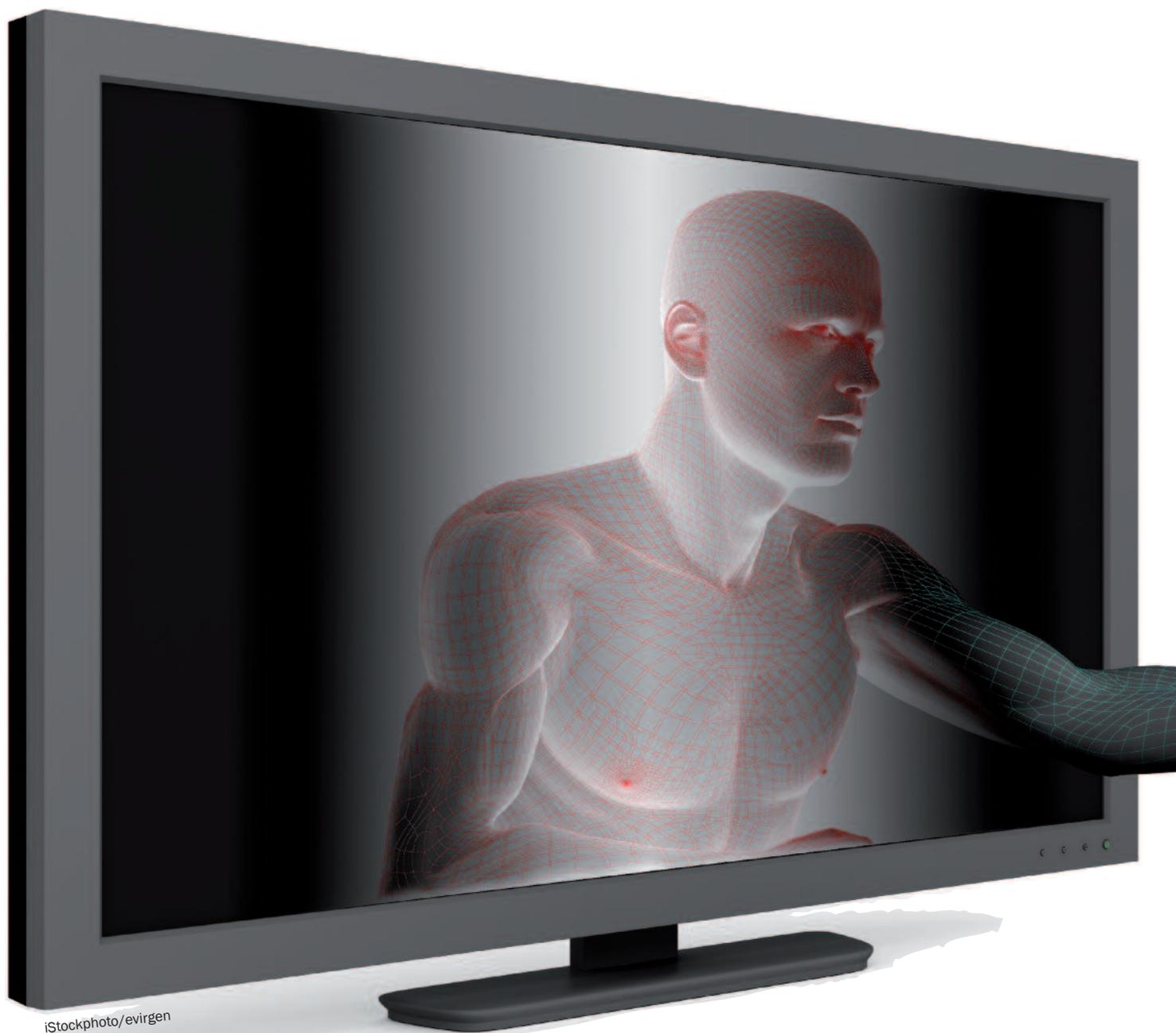


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# Chemistry in Second Life

## Part 1. A world of visualisation

BY ANDREW LANG AND JEAN-CLAUDE BRADLEY



iStockphoto/evirgen

The multi-user virtual environment of Second Life is not limited to the realms of role-play or romance. It can be a platform for the interactive and collaborative visualisation of molecules, spectra and experimental data.

With over 80 000 simultaneous users on at any given time, Second Life has emerged, according to their official statistics, as the most popular non-game-based 3D virtual world. Users interact with the environment and with each other in the form of avatars, usually lifelike representations of people or animals. Since users are empowered to create objects and environments of their choosing, almost every aspect of real life has been replicated in Second Life. Of course, since virtual worlds do not necessarily suffer the same limitations as reality, creative adaptations abound. Science is no exception and many exhibits in Second Life can be found depicting scientific content <<https://sites.google.com/site/slscgroupsite/home>>.

Chemistry presents some special challenges and opportunities for a platform like Second Life. Full use of 3D space is a real asset, since an understanding of the shape of molecules and orbitals is essential for chemists.



Such representations can be made in Second Life. Chemical data can also benefit from use of 3D space, for example in interactive exhibits.

## Molecules

Second Life provides an environment to interact with molecules in their full 3D representations. Only recently has it been possible to easily render molecules with realistic conformations. Our molecule rezzor, named Orac <<http://usefulchem.blogspot.com/2007/09/inchi-rezzer-in-second-life.html>>, is a tool that anyone can use to easily create molecules. (To 'rez' means to create or make an object appear in Second Life. A scripted object that rezzes other objects, such as molecules, is called a rezzer.)

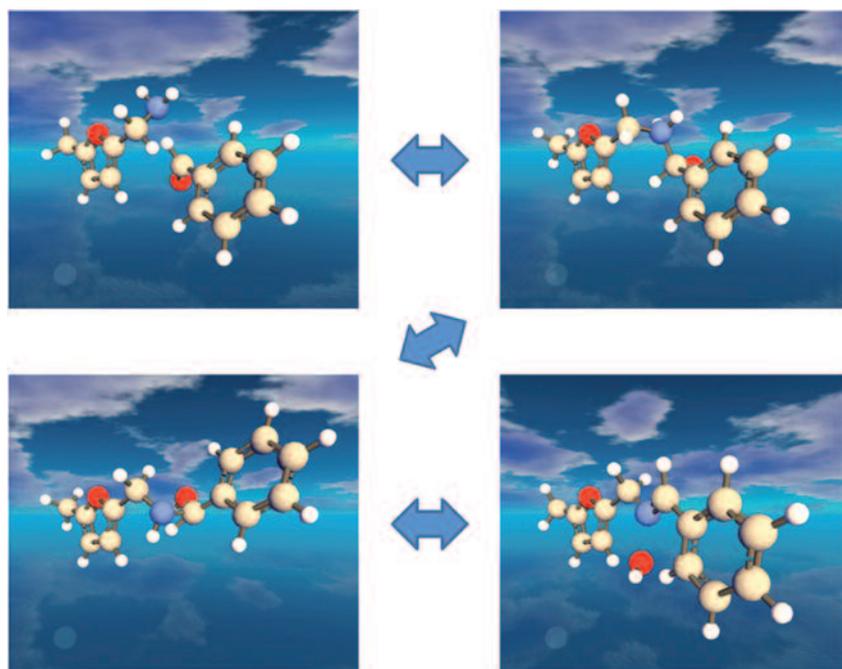
The molecules that Orac makes can be manipulated in many ways. You can easily change the position, size and orientation, you can save the molecules to your inventory for later retrieval, make multiple copies and even distribute them to other users.

Also, with a little scripting, you can make the molecules interact with users and even each other.

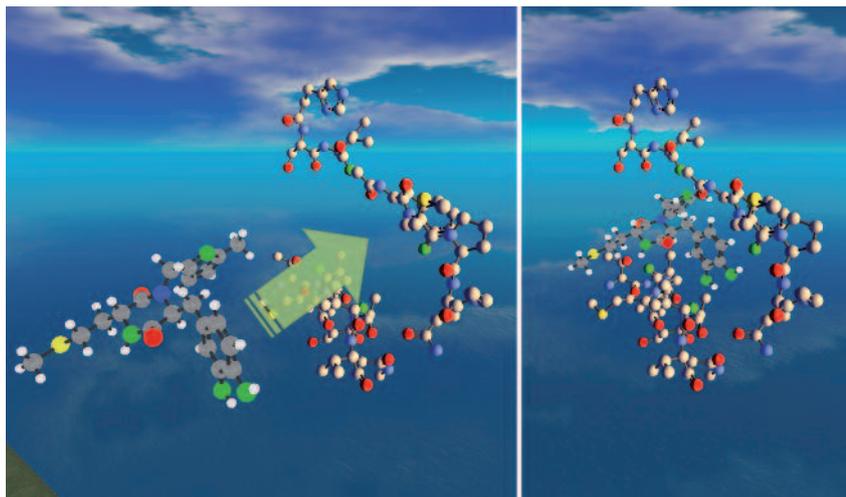
Orac uses freely available web services to dynamically calculate and display 3D molecular data.

## Reactions

Using Second Life, it is possible to render chemical reactions in full 3D <<http://drexel-coas-elearning.blogspot.com/2007/08/teaching-chemistry-mechansims-in-second.html>>. By scripting the atoms and bonds of molecules to respond to chat, users can step through a reaction mechanism by simply typing 'next' and 'back'. As the user commands the molecules, they see bonds twist, break and re-form as the atoms move to their new positions in each fully minimised intermediate structure. The image



Snapshots of each step in a user-controllable reaction mechanism simulation.



Molecule docking in Second Life.

shows snapshots of the reaction of benzaldehyde with 5-methylfurfuryl-amine to form an imine and water. Each intermediate in the reaction has been minimised to show a realistic conformation. Large changes in geometry are easily appreciated within the 3D environment, something that is not easily represented in 2D renderings on paper.

## Docking

Simple non-rigorous rigid docking, via hydrogen-bond contact points, can easily be implemented using Second Life's built-in scripting language. We scripted an example from real-life antimalarial research <<http://dx.doi.org/10.1038/npre.2008.2216.1>>, so that when a user clicks on the docked molecule it jumps out of the binding pocket to a random location but same orientation. It then self-docks back into the binding pocket of the targeted enzyme (enoyl reductase in this case) by minimising the simulated hydrogen-bond interaction energy. The four hydrogen-bonding interactions between the molecules and the atoms involved are tagged in green in the image above <<http://usefulchem.blogspot.com/2007/06/molecule-docking-in-second-life.html>>. To achieve a more realistic docking simulation, a docking web service could be used; and together

with human interaction, more efficient and sometimes better results (by avoiding local minima), over computer-only docking, can be achieved (see Subasi and Basdogan, *Teleoperators & Virtual Environments* 2008, **17**(1), 73–90).

## Peptides and proteins

Joan Slonczewski of Kenyon College in the US has created Amino World to help students identify amino acid R groups in peptides (see <http://daneelariantho.wordpress.com/2008/06/15/a-amino-world/>). Amino World consists of five peptides, each composed of four amino acid residues. The peptides of Amino World are fully interactive, complete with extensive information available on notecards that users can save to their inventories, and by clicking on the peptide tower controller or the molecule itself you can highlight different structures such as the peptide backbone and the different R groups. The R groups can be made to identify themselves and copies can be taken and examined by users.

Second Life has a few built-in limitations that currently make the rendering of large stick-and-ball molecules impractical. For example, there is a limit to the number of atoms that can be linked together to form a single molecule. Practically, this limit is

around 120 atoms for most molecules. Several solutions to these limitations have been developed.

One example is a protein rezzing toolkit developed by Peter Miller at the University of Liverpool in the UK, which gives users the ability to manage large protein structures in Second Life.

Paul Bourke of the University of Western Australia has done innovative work in evaluating Second Life for remote collaboration and visualisation, including chemistry visualisation. His work includes examples of immersive crystal structure visualisation, including Hershfield surfaces, using preprocessed spherical projections, a useful visualisation technique <<http://local.wasp.uwa.edu.au/~pbourke/papers/cgat08>>.

## Spectra

Second Life continues to improve its interoperability with the web and therefore its usefulness as a platform for interacting with all forms of media, including scientific data. One thing that is now possible is the ability to dynamically create images on any server and then have that image appear in Second Life for all to see. We have used this ability to build an interactive spectrum viewer <<http://usefulchem.blogspot.com/2008/04/nmr-viewer-in-second-life.html>>. The viewer interacts with users via chat and responds to commands such as 'zoom [range]', 'back' and 'reset'. By typing 'zoom' with a specified range of values, you can expand any area of the spectrum. The integral value is also calculated and displayed on the resulting image.

The particular spectrum shown can be changed from within Second Life by simply changing the Media URL to point to the appropriate spectrum file. Displaying spectra in Second Life has advantages over currently available web-based viewers: in addition to the inherent collaborative nature of Second Life, it is easier to control focus, it has the integral value and it

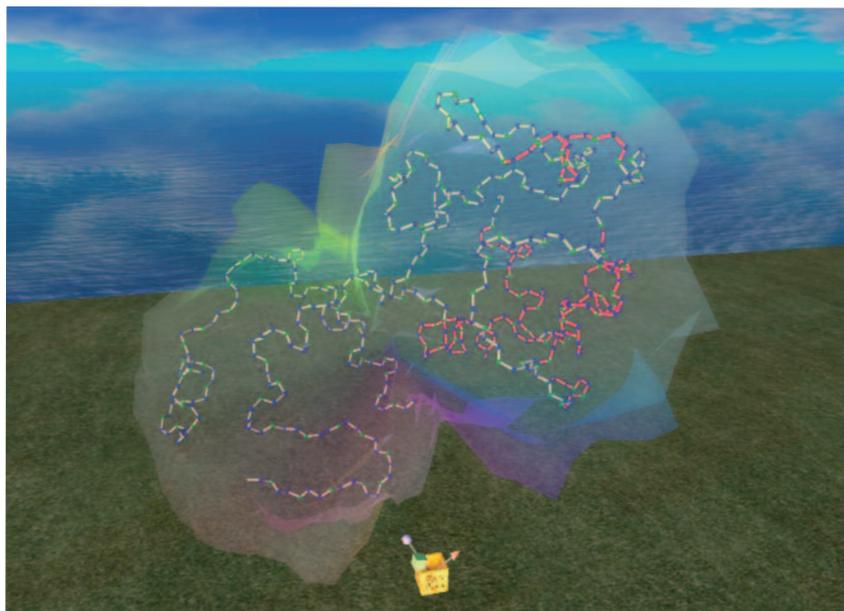
can be used in conjunction with other chemistry visualisation tools.

## Solubility

Our Ugi solubility explorer (Bradley et al. *Journal of Visualised Experiments* 2008, 942) is a data visualisation tool that allows users to select the four components of the Ugi reaction (an aldehyde, an amine, an isonitrile and a carboxylic acid) and view the solubility data for each compound in various solvents in a 3D bar chart.

Another way to view the solubility data as a whole is through an interactive descriptor chemical space <<http://usefulchem.blogspot.com/2009/01/interactive-visualization-of-ons.html>>, a real-time 5D visualisation of the solubility data. By clicking on any data point in Second Life, you again can access the solubility data for each experiment.

The solubility explorer and 5D chemical space rezzer allows us to explore the data in real time to find target solvents for particular combinations of Ugi reactants and analyse the chemical space for solubility trends. It also allows us to easily visualise regions of the data,



A protein (3cyt) rezzed using the protein rezzer toolkit enveloped in a sculpted protein.

seeing where the data is sparse, and guiding further research.

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The authors are experimenting with some Open Access alternatives to Second Life and replicating some of the chemistry there. Updates will be posted at <http://drexelisland.wikispaces.com>.



Ugi reaction solubility explorer.

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