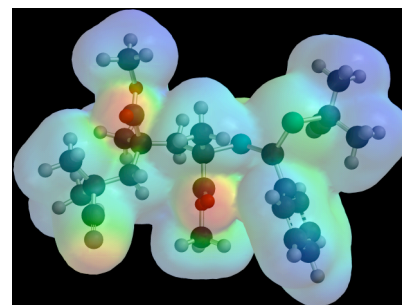


# Computational Chemistry Polymer Chemistry

*Associate Professor Michelle Coote*



We use computer calculations to determine the structure of molecules and to help understand how molecules react with one another. Using the laws of quantum mechanics, we can calculate from first principles the structures of molecules, their vibrational frequencies and their energies. This provides detailed information on the mechanisms of reactions, as well as calculations of their kinetics and thermodynamics. We use these calculations to solve chemical problems — Why does a reaction fail? How can we make it faster or more selective? How can we control the stereochemistry? ... etc. We can even predict the outcome of new chemical processes prior to experiment, and can design improved reagents *in silico*. We work closely with experimental groups who put our computational designs into practice, and are members of the *ARC Centre of Excellence for Free-Radical Chemistry and Biotechnology*.

## Projects for Summer 2009-2010

- *Chain Carriers for Organic Synthesis*. Computational chemistry will be used to develop a more general method for evaluating the thermodynamic performance of radical chain carriers for organic synthesis, relative to available alternatives and relative to the desired synthetic transformations.
- *Modeling Radical Polymerization Processes*. Computational chemistry will be used to study the mechanism by which Lewis acids induce stereocontrol over the propagation step in free-radical polymerization, with a view to developing new chiral auxiliaries to expand the scope of this process.
- *Radical Processes in Biological Systems*. Computational chemistry will be used to evaluate new antioxidants and study the mechanism by which they protect us from oxidative damage.

In each of these projects, our primary focus is to use computational chemistry as a research tool to study chemical problems, with the emphasis on using our data to clarify reaction mechanisms, interpret structure-reactivity trends and thereby design new improved reagents. The majority of our calculations are performed using commercially available quantum chemistry software, in conjunction with various in-house scripts. These are very easy to learn to use and a specific background in computational chemistry or quantum mechanics is *not* required.

## More Information:

Email: [mcoote@rsc.anu.edu.au](mailto:mcoote@rsc.anu.edu.au)

<http://rsc.anu.edu.au/research/coote.php>

[http://www.freeradical.org.au/index.php?option=com\\_content&task=view&id=51&Itemid=53](http://www.freeradical.org.au/index.php?option=com_content&task=view&id=51&Itemid=53)