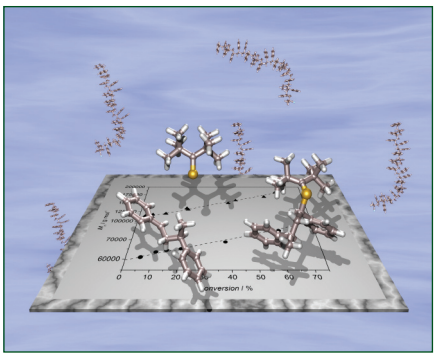
2005 RESEARCH HIGHLIGHTS

From Professor Peter Gill's group: The Hartree–Fock energy of a system is the energy that it would have if each electron felt only the average effect of all of the others. The error of the Hartree–Fock approximation is called the correlation energy E_c and, in order to predict chemical behaviour from quantum mechanical first principles, it is important to calculate E_c accurately. Traditionally, this has been very complicated and time-consuming but, recently, we made the radical proposal that E_c can be found relatively simply from knowledge of the positions and momenta of pairs of electrons in the system. Our first detailed discussion of this was chosen as a "Hot Article" in *Phys. Chem. Chem. Phys.* and was highlighted on the front cover of the first 2006 issue of that journal. As one reviewer wrote, *"Since really novel approaches to obtaining molecular energies arise only occasionally (the last one was probably density functional approximations), this is a potentially very exciting development."*

Ms Iris Li from Professor Chris Easton's group presented her work on the development of enzyme inhibitors to regulate the over-production of mammalian peptide hormones at the Gordon Conference on Free Radicals in New Hampshire, USA, and as a result of that presentation, was invited to present a lecture to the Conference. Gordon Conferences are for the top specialists in the field and only the top few percent of presentations are ever selected for invited lectures – so this was quite an honour for Iris.

Dr Michelle Coote and her group used computational chemistry to design the first multipurpose RAFT agents (fluorodithioformates), capable of controlling the polymerisation of monomers with disparate reactivities. Although designed entirely by computer they have subsequently been synthesised by collaborators at UNSW and demonstrated experimentally to control polymerisation. Computer-aided chemical design was also used to design a new route to polyphosphines and a new method for controlling free-radical polymerisation using thioketones as radical spin traps. The illustration (right) featured on the cover of Chemical Communications (Ah Toy A, Chaffey-Millar H, Davis T P, Stenzel M H, Izgorodina E I, Coote M L, Barner-Kowollik C, *Chem. Commun.* (2006) (8), 835-837, http://dx.doi.org/10.1039/b515561d and signifies their method for controlling free-radical polymerisation using thioketone spin traps.



A novel NMR spectroscopic technique was developed in the Otting/Keniry groups that allows the rapid determination of the three-dimensional (3D) structures of protein–protein complexes. The method starts from the known structures of the individual protein molecules (determined by previous X-ray or NMR studies) and uses the effects from paramagnetic lanthanide ions on the ^{1}H-NMR spectra to establish the relative orientation and positioning of the protein molecules with respect to each other. The attraction of the method lies in the fact that only a few NMR signals of each protein need to be assigned and that these assignments can be obtained in an automatic manner based on the 3D structures of the proteins and few NMR spectra recorded of selectively ^{15}N-labelled protein samples. The method was demonstrated with the complex of the ε and θ subunits of DNA polymerase III, whose structures had been determined separately in collaborations among the Keniry, Ollis, Dixon and Otting groups.