Theoretical and Computational Reactivity @ RSC

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I use mostly computational methods to study the dynamics of chemical reactions. While using significant amounts of computer time on the national supercomputers, this is generally not simply using established methods and existing programs to probe the reaction du jour. Though I do use existing packages on novel problems, the focus is developing methodology to study interesting reactive systems that are not readily accessible with current approaches. This ranges from the quantum dynamics of gas phase reactions to the energetics of solid state systems and, more recently, the interactions between gas phase species and solid materials that are quietly ubiquitous in science and technology.

Potential projects for 2014-15:

• **Reactions on interstellar ices.**  
The CO + H reaction lies at the beginning on a sequence of reactions leading to complex molecules in interstellar space. This reaction is thought to occur on the surface of CO-containing ice mantles, but is difficult to study experimentally. Current methods to model reactions such as these rely on assumed forms for the energies of interacting particles. This project will use *ab initio* methods combined with *systematic fragmentation* to probe the reaction profile of such gas-surface reactions to answer fundamental questions about the energetics and mechanism of interstellar HCO formation.

• **Venusian ozone and sulfur oxide reactions.**  
Levels of sulfur oxides in the atmosphere of Venus are poorly understood. Recent proposals to explain the observed abundances in the Venusian cloud layers rely on uncharacterised reactions involving ozone. In collaboration with researchers from RSPE and the Fenner School, this project will use high level *ab initio* methods to characterise such reactions in an attempt to establish the feasibility of such proposals.

• **Shepard interpolation of dipole functions.**  
Applications such as coherent control of molecular systems with laser pulses and photodissociation require knowledge of not only the potential energy surface as a function of molecular coordinates, but also the dipole moment across the whole range of molecular motion. Efficient ways to construct potential surfaces have been developed for decades. Dipole surface construction techniques lag far behind. In this project automated interpolation techniques will be developed to put dipole moment surface generation on the same footing as potential generation. This project has a strong programming and mathematical content.

• **Geometrical neighbour searching.**  
Over many years potential energy surface interpolation methods have been developed at ANU. The automatic treatment of polyatomic reaction systems is now routine, and modelling polyatomic adsorbates on crystalline surfaces is becoming so. The bottleneck for running calculations with these methods has become creating the “neighbour list” for points at which the potential needs to be evaluated. This project will use mathematical and computer science techniques to develop methods for fast neighbour searching, dramatically enhancing the usability of these state of the art interpolation techniques. This project has a strong programming and mathematical content.
- **Modelling amorphous silicon.**  
  Amorphous silicon is a cheaper material for making solar photovoltaic cells than its more common crystalline cousin. In its hydrogenated form it is subject to a poorly understood thermal and photoactive process known as the Staebler–Wronski effect. This project will use *ab initio* methods combined with *systematic fragmentation* to model the structure and energetics of amorphous silicon, investigating how hydrogen interacts with the silicon structure and possible thermally mediated processes that may contribute to the Staebler–Wronski effect.

*And many more...* Custom projects related to molecular potential energy surfaces, gas phase reaction dynamics, electronic structure theory, solid state structure and energetics, crystal defects, phonons, astrochemistry, collisional energy transfer, etc., can be developed to suit a student's interests.