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“Unexpected Ligand Effects in C-H and C-F Bond Activation”

Prof. Stuart MacGregor

Heriot-Watt University, Edinburgh(United Kingdom)

Friday 4th March, 2011. ICIQ Auditorium, 12 p.m.



Professional Career:

- BSc Honours (1988) and PhD (1992) University of Edinburgh (Advisors: Alan Welch and Lesley Yellowlees)
- **November 1992 – October 1994**:EPSRC/NATO Postdoctoral Fellow, Université de Paris-Sud, Orsay, France (with Odile Eisenstein)
- **January 1995 - March 1997**:Postdoctoral Fellow, Australian National University (with Graham Heath).
- **April 1997 to 2005**:Lecturer, Heriot-Watt University
- **August 2005**: Promoted to Reader
- **August 2008**:Promoted to Full Professor
- **Currently** Academic Head of Chemistry

Research:

The interests of their group lie in the use of computational modelling to understand the reactivity of organometallic complexes. The main results of their calculations are molecular structures and energies. Such information is especially valuable when not easily determined experimentally.

For example, in the lab the nature of the reactants and products is usually known, but determining the structures and relative energies of reactive intermediates and transition states is very difficult - yet it is often these species that determine the ease of a chemical reaction, or the degree of selectivity that a reaction may display.

Computational chemistry also provides the opportunity to relate the reactivity of a system to the underlying electronic structure - and may suggest new ways to enhance reactivity.