Thursday 10 March, 2pm (Ingram Lecture Theatre)

Timothy K Dickens (Cambridge)

Use of topology to understand molecular ring currents

Today computer programs such as Gaussian 09 are routine used to calculate properties of molecules. However many people using these programs have little understanding of what they actually do because they are so complex. This talk will explore paring back the mathematical models to some simple matrix mathematics and by by considering selective molecules constrained by geometry it is possible to gain fresh insight into patterns of chemical behaviour.