Electronic structure studies of the defect chemistry of TiO_2

Dr Benjamin J. Morgan and Prof. Graeme W. Watson
School of Chemistry, Trinity College, Dublin 2, Ireland.

Abstract

TiO_2 is one of the most widely investigated metal oxides, with numerous technological applications including photocatalysis of environmental pollutants, solar energy production, water splitting for hydrogen production, and possible spintronic devices. In all these cases crystalline defects can have large effects on the behaviour of experimental samples, and an understanding of both the relative stability of competing defects under variant synthesis conditions, and the effect of these on the electronic properties of the material, is necessary to optimise samples for real-world applications.

We will use high quality density functional theory calculations to study a range of intrinsic and extrinsic TiO_2 defects in both rutile and anatase. This will allow us to study the electronic and geometric structures of these competing defects, as well as their relative stability through calculating the formation energies. A detailed analysis of the electronic structure of comparable defects between the two polymorphs, rutile and anatase, will also be undertaken, to facilitate a greater understanding of the experimentally observed differences in photochemical behaviour.