PREDICTING the STRUCTURES and TUNING the ELECTRONIC PROPERTIES of INORGANIC POLYMORPHS

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Computer modelling now has a range of powerful techniques for predicting crystal structures[1] of both inorganic and organic materials. This lecture will first review the currently available techniques with examples of their application. We will then describe how the band structures of inorganic polymorphs may be accurately predicted for the topical example of TiO_2[2]. Here we will focus on the problem of the band alignment of the different polymorphs of this material and show how the relative positions of valence and conduction bands may be exploited to optimise the photo-activity of the material.

(1) Woodley SM and Catlow R, *Nature Materials,* **7**, 937, (2008)
(2) Scanlon D et al, *Nature Materials*, **12**, 798, (2013)