







Tight binding approximation for simulation of condensed matter

(two-part lecture)

Prof. Tony Paxton King's College London Part 1 (theory): Tuesday Aug. 11, 16:00, Room MXC 320 Part 2 (applications): Thursday Aug. 13, 16:00, Room MXC 320

Abstract: I would like to give a very personal account of the old and established tight binding approximation. Over the decades since 1954 this method comes in and out of fashion. In one year (1980) Volker Heine wrote "From Under a Cloud to out in the Sun". In 1985 he told me I was crazy to be doing it! P. W. Anderson first condemned the theory and then praised it. All along the quantum chemists have been using it under other names. It is probably the simplest quantum mechanical scheme that can account for bond breaking. In 1998 Mike Finnis and I invented the "self consistent polarisable-ion tight binding model" and 2008 we discovered "magnetic tight binding."

In the first lecture I will go over the theory, and in particular make contact where possible with the now very familiar density functional theory. I will finish with a brief mention of "time dependent tight binding" which was invented by Tchavdar Todorov.

In the second lecture I will give examples of its application from my own very recent research. I will talk about aqueous systems, and about carbon and hydrogen in iron and steel.