Tight binding simulations for solvent mixtures and chemical reactions

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Our self consistent polarisable ion tight binding model is in a sense an abstraction from the LMTO-Atomic Spheres Approximation because we use the unscreened structure constants to form the electrostatic potential energy of interaction of the multipole moments of the charge accumulated at each atom. However that it where the similarity ends, because this is an *empirical* scheme, like Walter Harrison's tight binding. We use quite a complicated genetic algorithm to fit the parameters of the model to a set of target data, taken from experiment or electronic structure. In fact we tend to avoid LSDA data as these do not describe the aqueous medium very well.

We now have a model set of parameters that describes the bonding, energetics and dynamics of both solvents and small molecules as well as the transition metal oxides, for which the model was originally designed.

In this poster I will show our latest, unpublished results.

M. W. Finnis, A. T. Paxton, M. Methfessel and M. van Schilfgaarde, *Phys. Rev. Letters*, **81**, 5149 (1998)