MATERIALS MODELLING; ADAPTING THE METHODOLOGY TO THE PROBLEM

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We review the respective roles of interatomic potential based and quantum mechanical methods in materials modelling and simulation. We identify classes of simulation, where potential based methods are still preferred tool. We then discusses their role in modelling complex multiconfigurational systems, where we focus on the topical case of the surface structure of zinc oxide and show how potential and DFT, methods may be effectively used in conjunction. We describe recent developments in hybrid QM/MM techniques and their application to the electronic structures of the polymorphs of titanium dioxide. Finally, we initiate a discussion as to how potential models may be improved and refined.