**Bond−order potentials : bridging the electronic to atomistic modelling hierarchies**

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Materials modelling is often contingent upon having reliable knowledge about the key mechanisms operating at the atomistic level. Unfortunately , however , in many materials systems of technological importance the results of atomistic simulations are questionable due to the unsatisfactory nature of the ’classical’ interatomic potentials used. This talk outlines the derivation of a novel class of interatomic potentials , the so−called bond−order potentials (BOPs) , which are obtained by coarse−graining the quantum−mechanical electronic structure within the chemically−intuitive tight−binding framework. The challenges to develop these ’quantum−mechanical’ interatomic potentials will be discussed with relation to simulating the growth of thin films and to understanding the defect behaviour in high−temperature intermetallics and fusion−reactor materials.