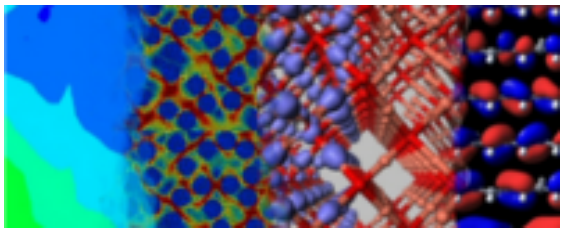

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Nanoscale materials and electronic transport: from ballistic to hopping approaches

Thursday, November 8, 2012 4:50 PM (25 minutes)

To support accelerating materials development cycles we have developed simulation approaches for de-novo characterisation and optimisation of materials and device properties with nanoscale constituents. In recent years we have developed simulation methods that describe the conformation and electronic properties of materials built on the basis of well-defined nanoscale constituents. We have applied these methods to describe both ballistic and hopping transport in nanoscale devices. Here we discuss applications on single-molecule electronics, specifically molecular wires (metallic, organic and DNA based) and on the development of an atomic transistor [1,2,3,4]. A second point of emphasis will be the development of methods to describe function of organic light emitting diodes [5] based on detailed atomistic models of their morphology and molecular properties, accent being on the morphology simulations with Monte Carlo methods. Finally I will discuss the integration of these methods into a European framework for multiscale materials modelling in the EU project MMM@HPC, which shall make these and other simulation method accessible to a wide audience of interested scientists and enable exploitation on high performance computing architectures.

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