Table of contents

Joint ICTP-IAEA Workshop on Physics of Radiation Effect and its Simulation for Non-Metallic Condensed Matter | (smr 2359)

Thursday 23 August 2012

Introduction to atomistic multi-scale modelling - Adriatico Guest House Giambiagi Lecture Hall (10:30-11:30)

In this lecture, ways in which the atomistic simulations can be extended both in space and in time will be described. For extensions in space, parallelisation methods will be described as well as how it is possible to link MD to finite element methods. However, the bulk of the lecture will be to describe the latest long time scale techniques by which the time scales of radiation effects can be extended from those accessible by classical MD. In MD the largest time step that can be used in a numerical integration scheme is of the order of 10-15s. Thus to simulate even 1s of real time would require 1015 integration steps which is computationally infeasible. To overcome this problem it is necessary to calculate the transition energy barriers between local minima on n-dimensional potential energy surfaces and the frequency of occurrence of such events. A review of the methods that can do this will be described. This will include methods that do not rely on a prior knowledge of what the transition may be. Such barriers can be used to determine diffusion coefficients required for rate theory models and implemented into on-the-fly kinetic Monte Carlo techniques.

time	title	presenter
10:30	Introduction to atomistic multi-scale modelling	ROGER SMITH