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

Tuesday 21 August 2012

Principles of classical atomistic molecular dynamics computer simulations - Adriatico Guest House Giambiagi Lecture Hall (09:00-10:00)

In this lecture I will describe the basic elements of the main techniques that are used to model ballistic collision phenomena in non-metallic condensed matter using classical molecular dynamics. Such simulations have been very successful at modelling the collisional processes and damage that can occur during the ballistic phase of a collision cascade.
The history of the subject will be discussed along with the way in which molecular dynamics simulations have developed from the first simulations carried out by Vineyard's group at Brookhaven in the early 1960's.
The main computer codes used in these simulations will be described along with details of the algorithms that are needed to implement the methods.
The topics will include a brief overview of numerical integration algorithms for Hamiltonian systems, temperature control, optimisation methods, numerical tricks that can speed up the simulations and the latest potential functions that are used, including variable charge potentials.

time	title	presenter
09:00	Principles of classical atomistic molecular dynamics computer simulations	ROGER SMITH