Consiglio Nazionale delle Ricerche
Istituto di Chimica dei Composti OrganoMetallici

Giovedì 14 Settembre 2017
alle ore 11.00

presso l'aula 2 dell'Edificio F
Area della Ricerca CNR
Via Madonna del Piano, 10 Sesto F.no (Firenze)

il Prof. Yuko OKAMOTO
Department of Physics, School of Science, Nagoya University
Japan

terrà il seguente seminario:

"Classical and quantum molecular simulations in generalized ensemble"

Dr. Giovanni La Penna
Primo Ricercatore

Dr. Francesco Vizza
Direttore

Abstract:

Conventional molecular simulations suffer from the multiple-minima problem where there are a huge number of local-minimum energy states in the system and the simulations tend to get trapped in some of these local-minimum states. In order to overcome this difficulty, we have been advocating the uses of the generalized-ensemble algorithms which perform random walks in potential energy and other physical quantities and their conjugate parameters. In this talk, I will give the latest results of our applications of generalized-ensemble algorithms to classical and quantum molecular simulations.

Biographic sketch:

http://www.tb.phys.nagoya-u.ac.jp/~okamoto/index-e.shtml