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VABILO NA INŠTITUTSKO PREDAVANJE / INVITATION TO THE INSTITUTE LECTURE

Dr. Fabio Pietrucci

Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

https://sites.google.com/site/fabiopietrucci

četrtek / Thursday, 29. 05. 2014, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

Reconstructing the thermodynamics and kinetics of activated processes with molecular dynamics simulations: from chemical reactions to biomolecular recognition

Abstract:

Molecular dynamics allows simulating a number of different physico-chemical processes at the experimental conditions of temperature, pressure, concentration, etc. Unfortunately, the time scale that is nowadays accessible is typically smaller than one nanosecond if interatomic forces are computed from density functional theory, or smaller than one millisecond if an atomistic force field is employed. Metadynamics [1] is an advanced technique designed to overcome this limitation: it greatly accelerates the sampling of the configuration space and it allows reconstructing the free energy profile, and sometimes even the kinetics, of complex activated processes occurring over time scales exceeding seconds. I will present the basic metadynamics algorithm and some recent developments.

On one side, it is possible to combine metadynamics with graph theory by regarding a system of atoms as a "social" network whose connections are the chemical bonds [2]. This approach allowed us to investigate complex multi-step chemical reactions without imposing any prejudice about the transformation pathway, leading us to rationalize the folding of a graphene flake into a fullerene-like cage observed by transmission electron microscopy [3], and opening the way to the systematic study of reactions in solution and phase transitions in disordered systems [4].

On the other side, to tackle very challenging biomolecular processes characterized by several different reaction coordinates, multiple metadynamics simulations can be run in parallel and their trajectories can be combined together to reconstruct high-dimensional free energy surfaces [5]. In this way we could investigate the detailed association mechanism of a substrate to HIV-1 protease [6], and the dimerization mechanism of the latter enzyme, discovering a promising new route towards the design of new drugs [7].

[1] A. Laio and M. Parrinello, Proc. Natl. Acad. Sci. USA 99, 12562 (2002).
[2] F. Pietrucci and W. Andreoni, Phys. Rev. Lett. 107, 085504 (2011).
[3] F. Pietrucci and W. Andreoni, J. Chem. Theory Comput. 10, 913 (2014).
[4] G. A. Gallet and F. Pietrucci, J. Chem. Phys. 139, 074101 (2013).
[5] F. Marinelli, F. Pietrucci, A. Laio, S. Piana, PLoS Comput. Biol. 5, e100045 (2009).
[6] F. Pietrucci, F. Marinelli, P. Carloni, A. Laio, J. Am. Chem. Soc. 131, 11811 (2009).
[7] F. Pietrucci and A. Kranjc, (to be submitted).

Vljudno vabljeni! / Kindly invited!

Info: Janez Mavri; janez.mavri@ki.si in Jernej Stare; Jernej.stare@ki.si