Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via R. Cozzi 55, 20125 Milano

February 10, 2022 – 2.30 p.m.

Seminar room - Department of Materials Science U5

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Enhancing Fluctuations along Kinetic Bottlenecks

Sampling Reactive Events in Catalysis

Molecular dynamics (MD) is a powerful tool to study the evolution of complex chemical systems. However, relevant metastable states, like reactants an products of a reaction, are often separated by large freeenergy barriers limiting the application of MD to the study of rare events. Enhanced sampling methods, like metadynamics, allow overcoming high free energy barriers, thus, favoring transitions among metastable states of interest. In this talk, I will focus on chemical reaction sampling, defining the rare events problem and the enhanced sampling solutions to it, from the choice of the biasing method to the selection of proper collective variables. Examples from realistic application problems of nanoconfined catalytic reactions will be presented, ranging from organic synthesis of pharmaceutical compounds in biomimetic calixarene capsules to heterogeneous biomass conversion over solid/liquid interfaces in zeolites.

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator

Prof. Marco Bernasconi