UNIVERSITÀ DEGLI STUDI DI PADOVA

DiSC

Lunedì **16 settembre 2019** alle ore **16:30** presso l'aula F

il Dott. Silvio Pipolo

Université de Lille, Unité de Catalyse et Chimie du Solide,
Lille, France

terrà il seminario dal titolo:

Simulating complex transformation in condensed matter

Simulating complex transformations of condensed matter like phase transitions or protein folding is a challenging task due to the big gap between the physical timescales the ones accessible to simulations. Among the different MD accelerating techniques, metadynamics [1] provides a powerful tool to overcome such limitation and to reconstruct the free-energy landscape.
The definition of a suitable collective variable tracking the transformation mechanism is the key problem and it is strongly process-dependent. Because, in general, these processes encompass both short-range chemical changes and long-range collective processes, finding good coordinates is highly non-trivial.
We propose a general coordinate that combines the Path Collective Variable (Path-CV) [2] and the Permutation Invariant Vector (PIV) [3, 4]. This allows to trace a continuous path between the initial and the final state in a two-dimensional space and accounts for the topological complexity of the structures through the PIV metrics. We apply such methodology to different phase transitions between crystalline and amorphous ice phases, exploring the mechanisms and energetics of the processes at different thermodynamics conditions (pressure and temperature) by computing free-energy barriers and transition paths [4,5].

[1] A. Laio and M. Parrinello, Proc Natl Acad Sci U S A. 99 12562 (2002).
[2] D. Baranduardi, F.L Gervasio and M. Parrinello, J. Chem. Phys. 126, 05410 (2007).
[3] G.A. Gallet and F. Pietrucci J. Chem. Phys. 139, 074101 (2013).
[4] S. Pipolo, G. Ferlat, M. Salanne, A.M. Saitta and F. Pietrucci PRL 119, 245701, (2017).
[5] M.Fitzner, G.C.Sosso, F.Pietrucci, S.Pipolo and A.Michaelides, Nature Comm. 8, 2257, (2017).

This seminar is supported by the EU H2020 ERC TAME-Plasmons project (ERC-CoG 681285)

Stefano Corni

Il Direttore del Dipartimento
Michele Maggini