UNIVERSITÀ
DEGLI STUDI DI TRIESTE

SEMINAR ANNOUNCEMENT

On **FRIDAY MAY 4TH 2018,**
at **11:00 am**, **in room "Sala del Consiglio" (I floor)**
of DSCF,
Trieste University, Building C11, Via Giorgieri 1

Prof. Devis Di Tommaso

School of Biological and Chemical Sciences and
Materials Research Institute
Queen Mary University of London
Will give a seminar entitled:

Modelling Processes of Crystal Growth and Nucleation from Solution

The seminar videoconference will be broadcast to University Ca' Foscari (Venice), at Sala Conferenze Orio Zanetto.

Everybody is kindly invited.

The Director

Prof. Silvano Geremia

Modelling Processes of Crystal Growth and Nucleation from Solution

Devis Di Tommaso

School of Biological and Chemical Sciences and Materials Research Institute, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom. Email: d.ditommaso@qmul.ac.uk

The crystallization of pure polymorphs of active pharmaceutical ingredients and biomineralization phenomena in aqueous natural environments are some of the processes that crucially depend on the nucleation and growth of the crystal from a dispersed and disordered phase. Despite its importance and multidisciplinary character, molecular details of the events surrounding the crystallization from solution (separation of solute and solvent molecules, the formation of clusters and nanophases, interaction at the solid-solution interface) are still partially understood. This talk will present recent work conducted in my group to theoretically characterize the mechanism of new phase formation, and the structure and energetics of the intermediates and precursor transient phases.

Since the process of surface-cation-dehydration governs the kinetics of the reactions occurring at mineral surfaces, such as adsorption and crystal growth, I will report on the quantification of solvent-exchange processes occurring at the mineral-water interface, including the effect of surface structure,[1] solution composition, [2] and nanoconfinement [3] on the reactivity of mineral surfaces.

I will then present analytical macroscopic geochemical models for describing mineral surface reactivity and predicting growth rates as a function of the surface topography that have been developed by "scaling up" molecular-level data obtained from molecular dynamics simulations of structurally heterogeneous mineral-solution interface.[4]

In the final part of the talk, I will describe a computational protocol to compute the free energy pathway for the formation of pre-nucleation molecular clusters in different solvation environments.[5] This methodology has been applied to rationalize the role of solvent in the self-assembly of *meta*-aminobenzoic acid, an important model system in the study of polymorphism and crystallization of active pharmaceutical ingredients.[6,7]

References

[1] M. Wolthers, D. Di Tommaso, Z. Du and N. H. de Leeuw, *Phys. Chem. Chem. Phys.*, 2012, **14**, 15145.
[2] D. Di Tommaso, E. Ruiz-Agudo, A. Putnis and C. V. Putnis, *Phys. Chem. Chem. Phys.*, 2014, **16**, 7772.
[4] M. Prakash, T. Lemaire, N. H. de Leeuw, M. Caruel, M. Lewerenz, D. Di Tommaso and S. Naili, *Phys. Chem. Miner*., 2017, **44**, 509.
[4] M. Wolthers, D. Di Tommaso, Z. Du and N. H. de Leeuw, *CrystEngComm*, 2013, **15**, 5506.
[5] D. Di Tommaso and K. L. Watson, *J. Phys. Chem. A*, 2014, **118**, 11098.
[6] E. Gaines, K. Maisuria and D. Di Tommaso, *CrystEngComm*, 2016, **18**, 2937.
[7] E. Gaines and D. Di Tommaso, *Pharmaceutics*, 2018, **10**, 12.