DIPARTIMENTO DI CHIMICA, BIOLOGIA E BIOTECNOLOGIE

UNIVERSITÀ DEGLI STUDI DI PERUGIA

PHD PROGRAMME IN CHEMICAL SCIENCES

Research seminars

Unraveling the mechanism of ice nucleation through rare events sampling and free energy calculations

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Many interesting physical processes occur on timescales that are very long compared to the shortest significant timescale involved. For example, timescales for folding the smallest of proteins are in the range of microseconds to milliseconds, while small-amplitude motions of amino acid side chains occur within 1 fs. This large difference of timescales can present serious computational challenges: 1 second of computational time (within one or two orders of magnitudes) would be needed to advance the simulation of 1 fs of physical time. Therefore, the investigation of processes like chemical reactions, diffusion in solids, protein folding, and nucleation processes require the use of rare events sampling methods. Here, I will demonstrate the suitability of rare events techniques to investigate the nucleation mechanism of ice. The freezing of water affects the processes that determine Earth's climate, therefore, accurate weather and climate forecasts hinge on good predictions of ice nucleation rates. Such rate predictions are based on extrapolations using classical nucleation theory (CNT). CNT assumes that the nucleation mechanism is one-step, that the reaction coordinate is the size of the critical nucleus and that the thermodynamic properties of the crystallite at the top of the barrier are the same as for the bulk. Transition path sampling and free energy calculations will be used to test these assumptions and to unravel the mechanistic pathways leading to ice nucleation in the atmosphere.

Tuesday, May 30, 2023, at 15:00

Room B (Via Elce di Sotto 8)

All interested are invited to participate.

Marco Paolantoni