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S E M I N A I R E

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« Advanced Sampling in Liquids »

Chemical potential is a key thermodynamic quantity in chemical physics, regulating a wide range of phenomena, such as phase transitions and chemical reactions.
In this talk I will focus on the numerical study of chemical potential in liquid solutions, addressing two long-standing challenges in atomistic simulations of liquids.
The first challenge is the accurate computation of the chemical potential in liquids, which is generally hampered by the poor sampling of particle insertion energies in dense fluids.
We address this problem by applying metadynamics to substantially enhance the sampling of the insertion energy, thus improving the efficiency and accuracy of our computations [1].
The second challenge concerns the control of the chemical potential during the simulation processes in solution. I will describe a technique for simulating crystal growth in a constant chemical potential environment. This is achieved by applying an external force on the solution molecules, depending on the composition of the liquid phase. This approach minimizes the finite size effects occurring in this kind of molecular simulations, allowing for the observation of a stationary regime of crystal growth [2].

1] Perego, C., Giberti, F. and Parrinello, M., Eur. Phys. J. Spec. Top. (2016) doi:10.1140/epjst/e2016-60094-x
[2] Perego, C. and Salvalaglio, M. and Parrinello, M., J. Chem. Phys., 142, 144113 (2015) doi:http://dx.doi.org/10.1063/1.4917200

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SALLE DE CONFERENCES