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**Theoretical approach to crystallization: foundations and application to proteins**[1]

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A fundamental issue in the modern study of phase transitions is the description of the process of nucleation, i.e. the choices of nucleation pathways. Proteins, in particular, are well-known to sometimes crystallize by passing through a meta-stable amorphous state and simulation and theory have shown that this is also true of many other systems. The issue also arises in the important case of polymorphic materials. In all cases, the goal is to understand which pathway is favored and how this is affected by the external control parameters. In this talk, I discuss a theoretical description of nucleation that allows for the direct determination of nucleation pathways and of their relative probability of realization that takes into account both thermodynamics and kinetic effects. It is based on a formulation of nucleation as a fundamentally non-equilibrium process and fully incorporates the effect of free-energy landscapes, determined e.g. via Density Functional Theory, in a consistent manner.

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