For years, X-ray crystallography has been used to obtain protein structures and understand biomolecules functions and properties. However, it requires the formation to sufficiently good crystal which can be sometimes hardly obtained. To enhance the crystallization rate and the resolution of the structure, new generations of molecular glue based on lanthanide complexes have been developed and commercialized by the Polyvalan Start up. These complexes increase the crystals quality and quantity for many proteins and can also be used *in cellulo*to drive the crystallisation of protein complexes, or in association with other structure determination approaches such as NMR. However, their mechanisms remain unknown. To understand them, we mix interaction studies at solid state (by X-Ray crystallography), in solution (by NMR) and using computational approaches based on all-atom molecular modelling.

In this presentation, I will present what can we learn about protein nucleation from these computational approaches. What are the preferential Xo4 binding site in solution? How protein mutations can impact these interactions? How Xo4 can help the protein-protein interaction? Through two examples AdkA and lysozyme, I will show what computational approaches can bring to the understanding of Xo4 binding mechanism on protein surfaces.