SFB/TRR 21 - Colloquium

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Protein dynamics II: going beyond reaction coordinates

Molecular dynamics simulations allow an atomistic understanding of protein conformational changes. The classical picture postulates the existence of a suitable reaction coordinate to monitor the transition, disentangling the starting and ending state as well as the barrier between them. Notwithstanding, it is difficult to find such a coordinate because of the many degrees of freedom involved and the presence of thermal fluctuations. Recently, a new arsenal of tools that make use of complex networks has emerged to characterize these problems. Transition networks allow a high resolution mapping of the underlying free-energy landscape without invoking arbitrarily chosen reaction coordinates, paving the way for an unbiased, quantitative description of protein conformational changes.

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