PHYSIKALISCHES KOLLOQUIUM

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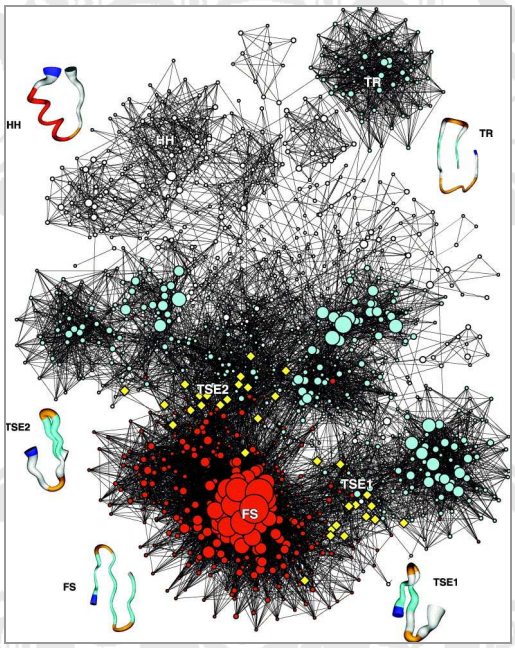
IM GROßEN HÖRSAAL



MOLECULAR DYNAMICS SIMULATIONS OF PROTEINS: ACHIEVEMENTS AND PERSPECTIVES

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Going back to Watson and Crick, the traditional structure-function paradigm, "to know function study structure", have guided our interpretation of protein function for decades. It is only rather recently that the role of dynamics has been recognized, supporting the idea that analysis of "static" structures is not sufficient to fully understand protein function. To this aim, molecular dynamics simulations are playing an increasing role in determining the mechanism, as a supplement to the experimental studies. To understand protein conformational changes, the classical picture postulates the existence of a suitable reaction coordinate to monitor the transition, disentangling the starting and ending states 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.