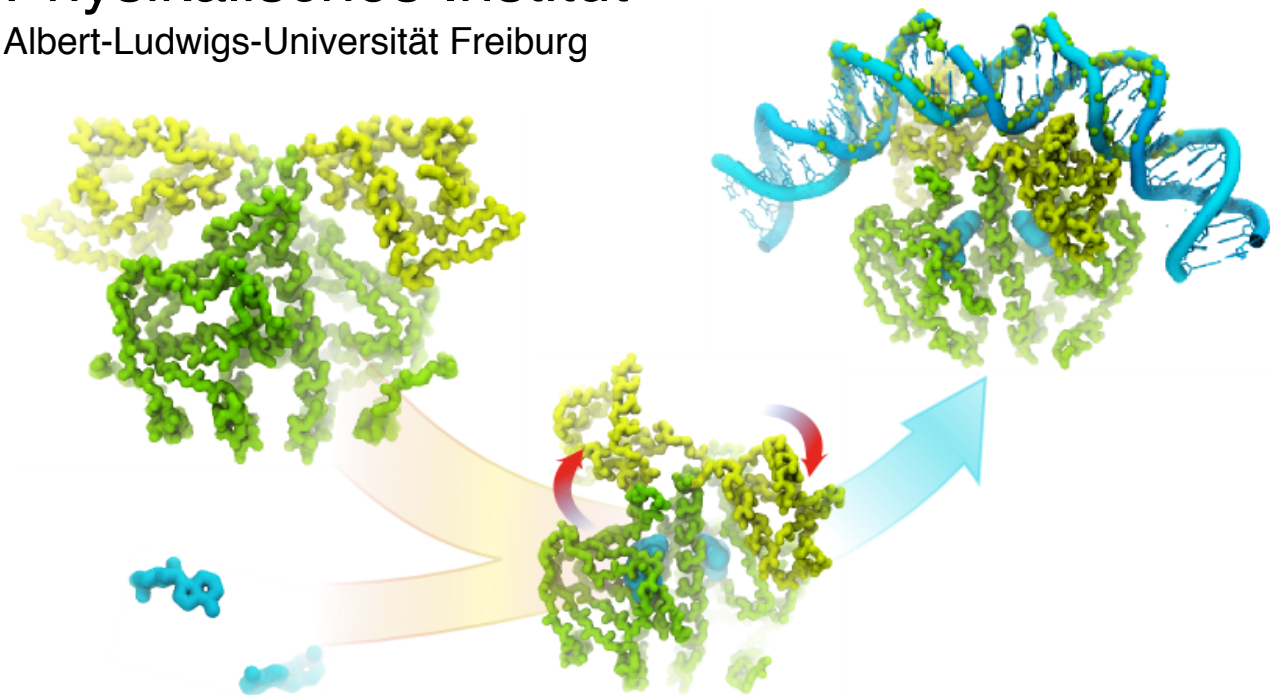
Physikalisches Institut

Albert-Ludwigs-Universität Freiburg



May 9

Rethinking molecular kinetics

Francesco Rao

FRIAS

Molecular conformational changes are conventionally studied in terms of a suitable chosen reaction coordinate, disentangling the reactant, the product and the barrier between them. In most real cases however, it is difficult to choose such a coordinate because the relevant degrees of freedom are a priori unknown. Recently, a new arsenal of tools has emerged as possible candidates to better characterize these problems, of which the formation and breaking of hydrogen bonds in water represents a prototypical example. We found that the fluctuations of inter-atomic distances take implicitly into account of the environment, paving the way for an unbiased, quantitative description of the molecular dynamics.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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