Reduced-Dimensional Models for Chemical Dynamics in Complex Environments

RIGOBERTO HERNANDEZ, ALEX V. POPOV, ELI HERSHKOVITS, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400 — Nonstationary Langevin models have been developed that are capable of capturing feedback between complex environments and the underlying molecular constructs which in turn collectively comprise the environment. Although initial justifications for this formalism were heuristic and phenomenological, in recent work we have shown that in some cases it arises as the projection of a simple model of a chemical system bilinearly coupled to a harmonic bath with a time-dependent coupling. Moreover, the stochastic model can be used to surmise the diffusion of a tagged particle in a colloidal suspension which swells or shrinks with time. Alternatively, a liquid crystal, modelled as a colloidal suspension of orientable bodies, can also exhibit driven (time-dependent) behavior by way of the rotation of a magnetic field. Once again, the diffusion of a tagged particle under such time-dependence, can be surmised by the stochastic model. Thus these models allow for a substantial reduction of the dimensionality of a complex environment while retaining its multiple-time-scale features.

Rigoberto Hernandez
School of Chemistry and Biochemistry, Georgia Institute of Technology
Atlanta, GA 30332-0400

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