

Bridging the time scale and length gap: from QM/MM to history-dependent metadynamics

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(Dated: July 22, 2003)

We introduce a novel method for exploring the properties of the multidimensional free energy surfaces of complex many-body systems. The method is based on the construction of a coarse-grained non-Markovian dynamics in the space defined by a few collective coordinates. The dynamics is biased by a history-dependent potential term that, in time, fills the minima in the free energy surface, allowing the efficient exploration and accurate determination of the free energy surface^{1,3}. We discuss the usefulness of this approach, that, combined with QM/MM², allows an accurate description of activated events in systems of large size. We will present results obtained applying the method to the study of oxidative damage in DNA⁴, structural phase transitions in solids⁵ and chemical reactions³.

REFERENCES

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