

# Overcoming the Time Scale Problem in Ab Initio Molecular Dynamics Simulations

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Ab initio molecular dynamics simulations have become a powerful tool in the investigation of physical, chemical and biological systems but one of their most serious limitations is the relatively short time scale of a few tens of pico seconds that can be covered. This clearly excludes the study of a large range of phenomena that lie outside this time window.

We have tested different acceleration techniques based on atomic or electronic bias potentials to extend these restrictive time limits and make the approach more efficient in the study of rare events.

By using selected terms of a classical force field as a bias potential multidimensional free energy surfaces can be calculated within the limited time scale of a first-principles molecular dynamics scheme. We present also a new method based on electronic bias potentials suitable for the acceleration of rare reactive events.