Ab Initio Path Integrals: Methods and Applications

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Ab initio path integrals are a generalization of Car−Parrinello molecular dynamics which allow to include also nuclear quantum effects [1]. Using intramolecular proton transfer involving significant rearrangements of the chemical bonds as an example [2], it is shown how to compute quantum free energy profiles for chemical processes using this method in conjunction with constrained molecular dynamics. The original method, however, allows only to compute time−averaged quantities by its very construction. Recently, this approach was combined with centroid molecular dynamics in order to get a glimpse of approximate quantum dynamics in complex systems [3].

[1] D. Marx and J. Hutter; *Ab Initio Molecular Dynamics: Theory and Implementation*, in *Modern Methods and Algorithms of Quantum Chemistry* pp. 301−449, Editor: J. Grotendorst (John von Neumann Institute for Computing, Forschungszentrum Jülich 2000), see
http://www.fz−juelich.de/nic−series/Volume1/marx.ps or .pdf

[2] M. E. Tuckerman and D. Marx, submitted.

[3] D. Marx, M. E. Tuckerman, and G. J. Martyna, Comput. Phys. Commun. **118**, 166−184 (1999).