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Molecular Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) method: an overview

Fabien Gatti[1*], Benjamin Lasorne[1] and Hans-Dieter Meyer[2]

[1]Institute Charles Gerhardt of Engineering, University of Montpellier, Montpellier 34095 France 3
[2]Department of Physical Chemistry, University of Heidelberg at Urbana-Champaign, Heidelberg, 67120, Germany

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We give a general presentation of the importance of including quantum effects involving the nuclei in chemistry, special emphasis being placed on wave-packet methods such as the MCTDH approach.

[1]. MCTDH stands for Multi Configuration Time Dependent Hartree. MCTDH is a general algorithm to solve the time-dependent Schrödinger equation for multidimensional dynamical systems consisting of distinguishable particles. MCTDH can thus determine the quantal motion of the nuclei of a molecular system evolving on one or several coupled electronic potential energy surfaces. Several illustrations are given in the context of experimental femtochemistry and attospectroscopy.

[2]. Examples including strong quantum effects (non-adiabatic photochemistry, use of quantum coherence to guide reactivity, tunneling, etc.) are shown. General perspectives for the future and possible technological applications are highlighted.

1. "Multidimensional Quantum Dynamics : MCTDH Theory and Applications", *Wiley-VCH* Edited by H.-D. Meyer, F. Gatti and G. Worth.

2. Editor : F. Gatti, "Molecular Quantum Dynamics. From Theory to Applications.," *in Physical Chemistry in Action Ed. Springer Verlag* 2014.

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