

UNDERSTANDING AND CONTROLLING CHEMICAL REACTIONS: APPLICATIONS OF THE MULTI-CONFIGURATION TIME-DEPENDENT HARTREE METHOD

F. Gatti¹, B. Lasorne¹, S. Guérin², D. Lauvergnat³, R. Marquardt⁴, H.-D. Meyer⁵

¹*Institut Charles Gerhardt, Université Montpellier 2, France, gatti@univ-montp2.fr*

²*OMR, Université Carnot de Bourgogne, France*

³*LCP, Université Paris-Sud, France,*

⁴*Institut de Chimie, Université de Strasbourg, France,*

⁵*Institute of Physical Chemistry, Universität Heidelberg, Germany*

We present several applications of the Multi-Configuration Time-Dependent Hartree method [1,2,3] to the understanding and the control of molecular processes involving quantum effects. We focus on diffusion rates of molecules on metal surfaces and processes guided by laser pulses, involving or not conical intersections, at the femto and sub-femto/atto time-scales.

[1] H.-D. Meyer, U. Manthe, and L.S. Cederbaum, *The multi-configurational time-dependent Hartree approach*. Chem. Phys. Lett. **165** (1990), 73.

[2] M. H. Beck, A. Jäckle, G. A. Worth and H.-D. Meyer, *The multiconfiguration time-dependent Hartree method: A highly efficient algorithm for propagating wavepackets*, Physics Reports **324** (2000), 1.

[3] H.-D. Meyer, F. Gatti, and G. A. Worth, editors, *Multidimensional Quantum Dynamics: MCTDH Theory and Applications.*, Wiley-VCH,(2009), Weinheim.