VIENNA COMPUTATIONAL MATERIALS LABORATORY

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# Theory for dynamics and control of ultrafast chemical reactions

A TALK BY L. González, Institute of Theoretical Chemistry, University of Vienna

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| DATE / TIME | 11.06.2012 , 04:00 p.m. (CET) |
| LOCATION | Josef-Stefan-Hörsaal, vormals kleiner Hörsaal der Materialphysik,<br>3. Stock, Boltzmanngasse 5/Strudelhofgasse 4 |
| ABSTRACT | In our group we aim at understanding chemical phenomena using contemporary computational and theoretical methods. In particular, we employ ab initio quantum chemistry to understand relationships between structure and function but we also develop reaction dynamical methods to model photochemical processes driven by light and even control chemical reactions using shaped laser pulses. For the latter purpose, we use quantum dynamical methods based on the time-dependent Schrödinger equation but also mixed quantum-classical methods, which while less accurate, allow considering simultaneously all the molecular degrees of freedom. Different applications of ultrafast photo-induced processes will be given. |