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TDDFT-based local control theory for chemical reactions IVANO TAVERNELLI, IBM Res Lab, BASILE F. E. CURCHOD, Department of Chemistry and the PULSE Institute, Stanford University, THOMAS J. PENFOLD, School of Chemistry, Newcastle University, Newcastle (UK) — In this talk I will describe the implementation of local control theory for laser pulse shaping within the framework of TDDFT-based nonadiabatic dynamics [1]. The method is based on a set of modified Tullys surface hopping equations and provides an efficient way to control the population of a selected reactive state of interest through the coupling with an external time-dependent electric field generated on-the-fly during the dynamics. This approach is applied to the investigation of the photoinduced intramolecular proton transfer reaction in 4-hydroxyacridine in gas phase and in solution [2]. The generated pulses reveal important information about the underlying excited-state nuclear dynamics highlighting the involvement of collective vibrational modes that would be neglected in studies performed on model systems. Finally, this approach can help to shed new light on the photophysics and photochemistry of complex molecular systems and guide the design of novel reaction paths.

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[2]B.F.E. Curchod, T. J Penfold, U. Rothlisberger, I.Tavernelli, Chem. Phys. Chem., 16, 2127, 2015

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