Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nonadiabatic dynamics with spin-orbit couplings GLORIA CAPANO, 2Laboratory of ultrafast spectroscopy, Ecole Polytechnique Fdrale de Lausanne, Lausanne, 1015, Switzerland., FELIPE FRANCO DE CARVALHO, 1Centre Europen de Calcul Aromique et Molculaire, Lausanne, 1015, Switzerland., IVANO TAVERNELLI, IBM Research Zurich, 8803 Rueschlikon, Switzerland. — In this talk I will present some recent advances in TDDFT-based nonadiabatic dynamics for molecular systems using Tullys surface hopping. In particular, I will describe a method for the efficient simulation of intersystem crossing events, which requires the on-the-fly calculation of spin-orbit coupling matrix elements along the trajectories. This approach will be applied to the study of the photophysics of metal-organic complexes in solution and of different carbon nanostructures including graphene nanoflakes and nanotubes with different wrapping topologies.

Ivano Tavernelli
IBM Res Lab

Date submitted: 06 Nov 2015 Electronic form version 1.4