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Real-time non-adiabatic modeling of time-resolved pump-probe spectra using time-dependent density functional theory ENRICO TAPAVICZA, TRAVIS THOMPSON, NOEL BALUYOT, WILBERTH NARVAEZ, CECILIA CISNEROS, NHI NGUYEN, California State University, Long Beach, OIVER SCHALK, Stockholm University, ROSEANNE SENSION, University of Michigan — We model non-adiabatic excited state decay of organic molecules using time-dependent density functional theory surface hopping [1,2]. Based on the surface hopping trajectories we compute time-resolved transient absorption spectra [3], time-dependent photoelectron ionization spectra [4], and time-depnednt circular dichroism spectra. Calculated spectra and molecular structures are used to unravel features in experimental spectra that are not directly accessible from experiments. Our trajectories allow to analyze parallel decay channels separately and asses the effect of substituents on the excited state decay and stereoselectivity of electrocyclic reactions. Applications include provitamin D and its model systems cyclohexadiene, alpha-terpinene, and phellandrene. [1] E. Tapavicza, A. M. Meyer, and F. Furche. Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. Phys. Chem. Chem. Phys., 13:20986, 2011. [2] E. Tapavicza, G. D. Bellchambers, J. C. Vincent, and F. Furche. Ab initio non-adiabatic molecular dynamics. Phys. Chem. Chem. Phys., 15:1833618348, 2013. [3] B. C. Arruda, J. Peng, B. Smith, K. G. Spears, and R. J. Sension. Photochemical ring-opening and ground state relaxation in alpha-terpinene with comparison to provitamin D3. J. Phys. Chem. B, 117(16):46964704, 2013. [4] Schalk, O.; Boguslavskiy, A. E.; Stolow, A. Two-Photon Excited State Dynamics of Dark Valence, Rydberg, and Superexcited States in 1,3-Butadiene. J. Phys. Chem. Lett., 5, 560-565, 2014.

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