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Classical nuclear dynamics on a single time-dependent potential in electronic non-adiabatic processes FEDERICA AGOSTINI, Max-Planck Institute of Microstructure Physics, ALI ABEDI, Hunter College of the City University of New York, YASUMITSU SUZUKI, National Institute of Advanced Industrial Science and Technology, SEUNG KYU MIN, Max-Planck Institute of Microstructure Physics, NEEPA T. MAITRA, Hunter College of the City University of New York, E.K.U. GROSS, Max-Planck Institute of Microstructure Physics — The Born-Oppenheimer (BO) approximation allows to visualize the coupled electron-nuclear dynamics in molecular systems as a set of nuclei moving on a single potential energy surface representing the effect of the electrons in a given eigenstate. Many interesting phenomena, however, such as vision or charge separation in organic photovoltaic materials, take place in conditions beyond its range of validity. Nevertheless, the basic construct of the adiabatic treatment, the BO potential energy surfaces, is employed to describe non-adiabatic processes and the full problem is represented in terms of adiabatic states and transitions among them in regions of strong non-adiabatic coupling. But the concept of single potential energy is lost. The alternative point of view [1] arising in the framework of the exact factorization of the electron-nuclear wave function [2] will be presented. A single, time-dependent, potential energy provides the force [3] driving the nuclear motion and is adopted as starting point for the development of quantum-classical [4] approximations to the full quantum mechanical problem. [1] Phys. Rev. Lett. 110 263001 (2013); [2] Phys. Rev. Lett. 105 123002 (2010); [3] Mol. Phys. 111 3625 (2013); [4] Europhys. Lett. 106 33001 (2014).

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