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Non-Adiabatic Molecular Dynamics with Conditional Wave Functions — •Guillermo Albareda[1], Heiko Appel[1], Ignacio Franco[2], Ali Abedi[3], and Angel Rubio[1,4] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany — [2]Chemistry Department, University of Rochester, USA — [3]Max-Planck Institut für Mikrostrukturphysik, Germany — [4]Nano-Bio Spectroscopy group and ETSF Scientific Development Center, Spain

A rigorous trajectory-based approach to treat the coupled electron-nuclear motion in terms of conditional wave functions is presented. By projecting the Schrödinger equation on the actual configuration of an infinite set of nuclear trajectories, an ensemble of conditional electronic equations of motion is obtained. These equations do not rely on any tracing-out of degrees of freedom and their propagation does not require a prior knowledge of the involved potential-energy surfaces. Using an exact factorization of the full molecular wave function, we establish a formal connection with the recently proposed exact potential energy surfaces [1]. This connection is used to gain insight from a simplified propagation scheme, which is demonstrated to capture non-adiabatic dynamics accurately in the limit of weak nuclear splitting. For pronounced branchings, we show how this simple algorithm partially captures dynamical steps between adiabatic surfaces [2] and discuss a route to improve the method. [1] A. Abedi, N. T. Maitra, and E. K. U. Gross, Phys. Rev. Lett. **105**, 123002 (2010). [2] A. Abedi, F. Agostini, Y. Suzuki, and E. K. U. Gross, Phys. Rev. Lett. **110**, 263001 (2013).

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Email: albareda@fhi-berlin.mpg.de