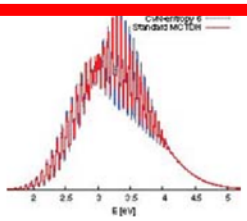
The Journal of Chemical Physics Editors' Choice for 2012

The Editors at *The Journal of Chemical Physics* facilitate publication of the most innovative and influential articles in the field of Chemical Physics each year. In the following collection, the Editors have selected a few of the many notable JCP articles published in 2012 that present ground-breaking research. This collection represents only a small fraction of the critical research published in JCP in 2012 and is representative of the broad cross-section of topics that the journal covers. These seminal articles are freely available online until the end of 2013. Download the entire list.

Section:

SPECIAL TOPIC: Nonadiabatic Dynamics



Till Westermann and Uwe Manthe

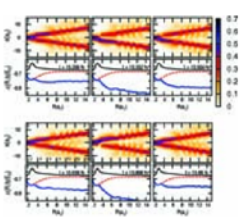
First principle nonlinear quantum dynamics using a correlation-based von Neumann entropy

J. Chem. Phys. 136, 204116 (2012)

Decoherence induced by conical intersections: complexity constrained quantum dynamics of photoexcited pyrazine

J. Chem. Phys. 137, 22A509 (2012)

In the first of a pair of papers, the authors introduce a new concept to describe the quantum dynamics in complex systems that extends established schemes based on the Dirac-Frenkel variation principle, e.g., the multi-configurational time-dependent Hartree (MCTDH) approach. They then extend the method—which uses a correlation-based von Neumann entropy (CvN-entropy) definition measuring the complexity of the wavefunction—to study decoherence effects induced by conical intersections, in particular, in the $S_0 \rightarrow S_2$ excitation in pyrazine. Investigating the CvN entropy after the $S_0 \rightarrow S_2$ excitation as a function of time, they obtain a clear separation of time scales related to the different dynamical phenomena present. Employing CvN-entropy constrained calculations, they analyze in detail the sensitivity of the autocorrelation function, the absorption spectrum, and the diabatic electronic population dynamics to complexity constraints.



Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction
Ali Abedi, Neepa T. Maitra, and E. K. U. Gross

In previous work, the authors showed that the complete wavefunction for a system of electrons and nuclei evolving in a time-dependent external potential can be exactly factorized into electronic and nuclear wavefunctions. The concepts of an exact time-dependent potential energy surface and exact time-dependent vector potential emerge from the formalism. Here, a detailed description of the formalism is presented, including a full derivation of the equations satisfied by the electronic and nuclear wavefunctions, and its relationshp to the traditional Born-Oppenheimer expansion is demonstrated.

J. Chem. Phys. 137, 22A530 (2012)