# View Abstract

**CONTROL ID:** 3496310
**TITLE:** Vibronic Spectra from First Principles: Capturing the Franck-Condon Effect without Born-Oppenheimer Surfaces
**Abstract Body:** We simulate electron-nuclear vibronic spectra using the semiclassical Multi-Trajectory Ehrenfest (MTEF) dynamics method, without relying on the use of excited Born Oppenheimer (BO) energy surfaces. We find that the vibrational energy spectra matches the energy profile of the initial state of the electronic system. We explore the roles of both the initial state preparation and the approximate semiclassical time evolution, and show how the MTEF approach allows for the inclusion of electron-nuclear correlation in the initial conditions. We apply this approach to a one-dimensional model for the Hydrogen molecule and with an ab initio treatment of Benzene using time-dependent density functional theory, demonstrating that this first principles approach, besides being efficient and scalable, performs well in comparison with experiment. These results show promise for the applicability of this real-time method to capture electron-nuclear correlated phenomena in time-resolved spectra, and in nonlinear driving regimes, for systems where the BO framework is computationally intractable.
**Funding Acknowledgement:** We acknowledge funding from the ERC through the QSpec-NewMat Project
**Special Instructions:** My collaborator Guillermo Albareda and I would like to present our talks in the same session, preferably back to back. His submission is entitled: "Conditional wavefunction approach to the structure and dynamics of quantum many-body systems."
**PRESENTATION TYPE:** Oral
**UNIT:** 16.0 GENERAL THEORY, COMPUTATIONAL PHYSICS (DCOMP)
**SORTING CATEGORY:** 16.01.04 First-principles modeling of excited-state phenomena in materials (DCOMP, DCP, DMP) [same as 05.01.14]
**Category Type:** Computational
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