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Abstract for an Invited Paper  
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**Photoexcited Nuclear Dynamics with Ab Initio Electronic Structure Theory: Is TD-DFT Ready  
For the Challenge?**

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In this talk, I will give a broad overview of our work in nonadiabatic dynamics, i.e. the dynamics of strongly coupled nuclear-electronic motion whereby the relaxation of a photo-excited electron leads to the heating up of phonons. I will briefly discuss how to model such nuclear motion beyond mean field theory. Armed with the proper framework, I will then focus on how to calculate one flavor of electron-phonon couplings, known as derivative couplings in the chemical literature. Derivative couplings are the matrix elements that couple adiabatic electronic states within the Born-Oppenheimer treatment, and I will show that these matrix elements show spurious poles using formal (frequency-independent) time-dependent density functional theory. To correct this TD-DFT failure, a simple approximation will be proposed and evaluated. Finally, time permitting, I will show some ab initio calculations whereby one can use TD-DFT derivative couplings to study electronic relaxation through a conical intersection.