

Abstract Submitted
for the DAMOP16 Meeting of
The American Physical Society

Quantum Dynamics Simulations for Modeling Experimental Pump-Probe Measurements BRETT PEARSON, SAHIL NAYYAR, KYLE LISS, Dickinson College, THOMAS WEINACHT, Stony Brook University — Time-resolved studies of quantum dynamics have benefited greatly from developments in ultrafast table-top and free electron lasers. Advances in computer software and hardware have lowered the barrier for performing calculations such that relatively simple simulations allow for direct comparison with experimental results. We describe here a set of quantum dynamics calculations in low-dimensional molecular systems. The calculations incorporate coupled electronic-nuclear dynamics, including two interactions with an applied field and nuclear wave packet propagation. The simulations were written and carried out by undergraduates as part of a senior research project, with the specific goal of allowing for detailed interpretation of experimental pump-probe data (in addition to the pedagogical value).

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Date submitted: 26 Jan 2016

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