DAMOP20-2020-000395

Abstract for an Invited Paper
for the DAMOP20 Meeting of
the American Physical Society

Monitoring Conical Intersections in Uracil by Ultrafast X ray Pulses

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Novel free electron laser X-Ray sources open powerful and unique measurement windows into ultrafast molecular dynamics. Using a realistic and fully ab-initio molecular Hamiltonian, we demonstrate the direct probing of coherences at conical intersections using X-Ray stimulated Raman signals. The signal is visible only at times where the wavepacket is in vicinity of the conical intersection. The wavepacket coherences survive for several hundred femtoseconds. Fundamental features such as wavepacket locality, conical intersection energy splitting and coherence duration in uracil can be directly accessed from the recorded signal. Our data set allows us to explore a vast parameter space affecting the signal: X-Ray probe wavelengths spanning several hundred electron volts, optimal probe bandwidths, and different molecular orientations and isotropic contributions. This gives a solid background for potential experimental realization. Resonant signals that probe the dynamics in the vicinity of a selected atom are presented and optimized using coherent control schemes.