

# PHYSICAL CHEMISTRY SEMINAR

**Wednesday, January 24, 2024  
10:30-11:30 a.m. BRWN 4102**

## *"Imaging Molecular Dynamics by Quantum Tomography"*



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#### Abstract:

Femtosecond and attosecond laser pulses provide the opportunity to image the motion of photoexcited molecular electrons. Since an isolated molecule is randomly orientated, this goal amounts to determining the evolving electronic probability distribution for every molecular orientation; which in turn requires the time and orientation dependent electronic density matrix. We present the determination of this Lab Frame Density Matrix in the photoexcited, rotating ammonia molecule, which we then use to determine the evolving electronic probability density at various orientations as well the time dependent orientation probability density which maps the rotational motion. We find that the rotational motion of the molecules drives charge migration across the molecule in different directions at different orientations. Finally, we discuss possible extensions of quantum tomography to rotating-vibrating molecules.



Department of Chemistry