CUNY NANO DAY

THURSDAY JUNE 15
CUNY ASRC

**3.00 pm** **A Structural Model of Nitro-Porphyrin Dyes based on Spectroscopy and Density Functional Theory**

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Nitro-porphyrins are an important class of commercial dyes with a range of potential applications. The nitro group is known to dramatically affect the photophysics of the porphyrin, but there are few systematic investigations of the contributing factors. To address this deficiency, we present spectroscopic studies of a series of nitro-porphyrins, accompanied by density functional theory calculations to elucidate their structures. In particular, we explore how the position of the substituent affects the energy levels and nuclear geometry. As expected, nitro groups on the meso-phenyl rings cause small changes to the orbital energies by induction, while those at the β-pyrrole positions more strongly conjugate into the aromatic system. In addition, however, we find evidence that β-pyrrole nitro groups distort the porphyrin, creating two non-planar conformations with distinct properties. This unexpected result helps explain the anomalous photophysics of nitro-porphyrins reported throughout the literature, including inhomogeneous line broadening and biexponential fluorescence decay.