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Angular Momentum Coherences in Vibrational Molecular Dynamics ZOE RAFTER, VARUN MAKHIJA, University of Mary Washington — Molecular dynamics describes what happens inside of a molecule (clump of atoms) after some amount of energy is dumped into a system, for instance when light is absorbed by a molecule. In natural systems, this absorbed energy often needs to transfer locations. The vibration of atoms in a molecule is believed to facilitate this transfer. In a particular excited state of the molecule of Nitrogen Dioxide (NO2), the bending and stretching of bonds is known to transfer energy from one vibrational state to another. This energy transfer is called Fermi Resonance. One potential way to image this vibration of a molecule is using ultrashort laser pulses. Ultrashort laser pulses last approximately a millionth of a billionth of a second, and act as a very short "flash" of a camera, during which the vibrations of the molecule are frozen. Such an experiment was recently attempted; however, the molecules were arbitrarily oriented and angular momentum was not considered. This arbitrary orientation effectively "blurs" the image. To remove this "blur", a calculation of the excitation step, including angular momentum must be carried out. Therefore, we include the angular momentum states of NO2 and computationally simulate the vibrational motion including angular momentum in the excited state.

Zoe Rafter
University of Mary Washington

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