NON-COVALENT DYNAMICS WITH A FEMTOSECOND LASER MOLECULAR BEAM MASS SPECTROMETER

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At Berkeley lab we are developing a versatile mass spectrometer to probe spectroscopic and time-resolved chemical dynamics involving non-covalent interactions. We are interested in the dynamic interactions of water weakly bound to hydrophobic molecular substrates (water in confinement).[1] Despite the cold conditions used to produce such complexes, they still retain large amounts of flexibility. Related are solvent-molecule rearrangements. Solvation can have a strong influence on chemical properties, and of particular interest is solvent dynamics as response to a stimulus, such as photoexcitation.[2]

Within the framework of astrochemistry, dynamics in larger molecules or their van der Waals clusters are largely unexplored. Processes that occur upon (V)UV radiation such as dehydrogenation, fragmentation, and ionization will be explored with the new laser system. Moreover, the tunability and high repetition rate of the UV/VIS pulses allows for fast electronic spectroscopy of reaction products for identification but also to spectroscopically characterize possible candidates for the diffuse interstellar bands.

The system will use 35% of the output from a 300 fs Yb fiber laser for generating the 115 nm ninth harmonic by a phase matched process of the third harmonic in a Xenon gas cell, running at up to 750 kHz.[3] The remaining 65% is used to pump an OPA that covers a tuning range of 210 nm to 16 μm. The resulting wide spectral range allows for direct ionization as well as electronic and vibrational spectroscopy of gas phase systems. The combination with short laser pulses allows for the characterization of fast structural and/or electronic changes upon excitation, ideal for tracking the dynamics of non-covalent systems.

1. Molina, E. R., et al. (2022), PCCP, 24(38), 23106-23118.
2. Miyazaki, M., et al. (2018), PCCP, 20(5), 3079-3091.
3. Peli, S., et al. (2019), arXiv preprint arXiv:1911.05590.