The Terahertz Dance

Shedding light on macroscopic systems one molecule at a time is the mission for DTU Chemistry's Assistant Professor René Wugt Larsen. With the prestigious Sapere Aude Grant he has set out to build a novel experimental platform for complementary spectroscopic experiments at DTU.

Assistant Professor René Wugt Larsen from DTU Chemistry became one of the chosen few when he received the Sapere Aude grant from The Danish Council for Independent Research Programme for the project entitled "Shedding Light on Macroscopic Systems One Molecule at a Time: Spectroscopy of Weakly Bound Cluster Molecules". The grant was given to support his efforts in shedding light on macroscopic systems one molecule at a time, an almost poetic mission considering that Kant coined the old quote Sapere Aude or "Dare to Be Right" as the essence of the Enlightenment.

"It is a great honor to receive this Sapere Aude Grant", René Wugt Larsen states. "It gives me the opportunity to found a research group with young, talented researchers and build a novel experimental platform for complementary spectroscopic experiments at DTU Chemistry."

New Spectroscopy Laboratory

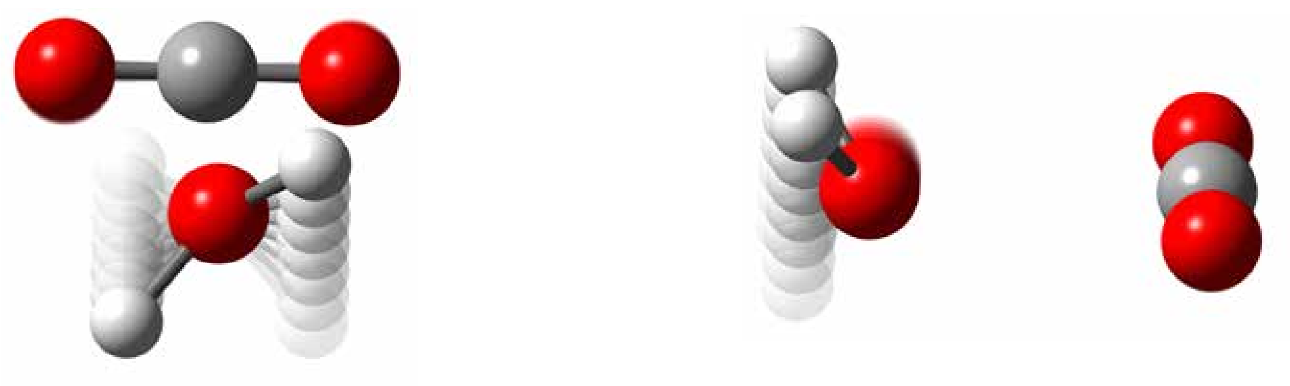
The research group consists so far of René Wugt Larsen and PhD students Jonas Andersen and Denise W. Mahler. A Post Doc arrives early 2014. They are setting up a new laboratory dedicated to studies of weakly bound molecular assemblies by a variety of novel experimental approaches based on THz and IR spectroscopy.

"One of the major challenges in the physical sciences is to explore how remarkable macroscopic properties of condensed bulk phases, materials and biological systems emerge from hydrogen bonding, dispersion interactions and steric repulsion between molecules at the microscopic level. The interplay between these classes of non-covalent forces emerges already on the nanoscopic scale of isolated molecular assemblies" says René Wugt Larsen.

"Dancing" Molecules

When two or more molecules approach one another they might eventually end up in a chemical reaction. However, in the course of their interaction the molecules will start vibrating collectively at THz frequencies and every such "THz dance" by a specific assembly of molecules has its own unique characteristics. This kind of characteristic intermolecular vibrational motion provides a wealth of information about the non-covalent interactions between the molecules and can help to describe similar, but structural more complex supramolecular systems e. g. natural gas hydrates, functional polymers and enzyme-substrate complexes of relevance to the energy, materials and life sciences.

"Modern quantum mechanical methodologies are able to describe these non-covalent interactions, but the methods scale fast with the number of electrons involved," René Wugt Larsen explains. In consequence, an accurate description of many relevant supramolecular systems is out of reach - even with the largest computer facilities. But if one can isolate and characterize the smallest molecular constituents on the nano scale level, molecule by molecule, it becomes possible to describe and spectroscopically characterize the specific forces involved.



Dancing molecules: The large-amplitude intermolecular vibrational motion associated with torsional motion, out-of-plane wagging and in-plane rocking of one single H_2O molecule interacting with one single CO_2 molecule.

And this is where the cluster spectroscopy research group rushes to the rescue. "In popular terms, we are going to shed light on macroscopic systems one molecule at a time," the group explain.

Building Solutions

In a current collaboration with Universität Göttingen, René Wugt Larsen and his group investigate the microscopic origin of the thermodynamical anomalies observed for bulk alcohol/water mixtures. It is well-known, that significant heat is released when mixing alcohol and water with a larger heat release for water-rich mixtures. They have been able to demonstrate spectroscopically that these macroscopic anomalies, to a large extent, originate from the relative stability of smaller hydrogen-bonded assemblies of alcohol and water molecules in the bulk liquids.

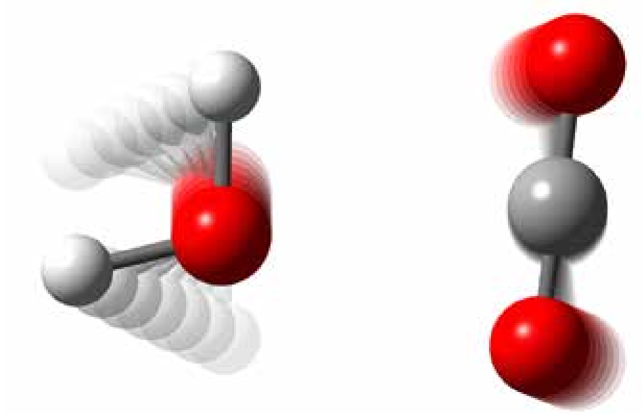
International Network

With a background in elite research groups at UC Berkeley, MAX-lab Storage Ring and Universität Göttingen, René Wugt Larsen has a strong network, and he intends to use the new cluster spectroscopy platform to strengthen DTU's international contacts even more:

"An important part of this project is to transfer knowledge of novel experimental facilities from Germany and Sweden to DTU Chemistry. The goal is to build up a variety of experimental setups, where weakly bound molecular assemblies can be trapped in inert cryogenic matrices or adiabatically cooled in supersonic free jet expansions at ultra-low temperatures," he explains. "In this way we are able to "freeze" the molecules' internal degrees of freedom and let them interact under controlled conditions synchronized with the spectroscopic experiment."

Since his days as a PhD student in Lund, René Wugt Larsen has maintained strong connections and a close collaboration with the MAX-lab Storage Ring in Lund. MAX-lab is a world-class facility for research based on highly brilliant synchrotron radiation. The facility is now to be extended with MAX IV, which will place Lund at the very top of international research and technology.

"I hope very much to establish a firm relationship and network between our cluster spectroscopy research group and the international research hub at MAX IV and the research community that will grow around it," says René Wugt Larsen.



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