Computational chemist computes to understand hydrogen bonds

Janet E. Del Bene, Ph.D., professor emeritus of chemistry at Youngstown State University, has relied on the Ohio Supercomputer Center since its inception in 1987 for her research in quantum theoretical chemistry.

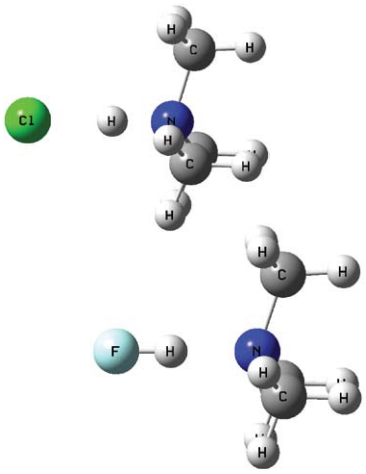
"As a computational chemist, my laboratory is the computer," said Dr. Del Bene, an expert in hydrogen bonding. Hydrogen bonds are responsible for the properties of water. Because most chemical reactions occur in water, chemists need to understand how hydrogen bonds influence chemical reactions.

Dr. Del Bene has addressed questions concerning the stabilities of hydrogen-bonded complexes, the methodological dependence of their computed properties, and has connected their infrared (IR) spectrosopic properties to the type of hydrogen bond present. Her work resolved what appeared to be a contradiction between theory and experiment in the description of certain types of hydrogen bonds.

Most recently, she has focused on how nuclear magnetic resonance (NMR) spectroscopy can be used to extract structural information about hydrogen bonds. By computing magnetic properties that can be measured experimentally in an NMR spectrum, Dr. Del Bene developed a way to characterize hydrogen bonds from their spectra and to obtain structural data for hydrogen-bonded systems in solution. Through her work, Dr. Del Bene and her colleagues have developed the chemical equivalent of infrared and nuclear magnetic resonance spectroscopic fingerprints of hydrogen bonds.

So what is the ultimate purpose of this work? Computational chemistry leads to a better understanding of chemistry and chemical reactions, and that understanding is the key to progress. ■

below: Hydrogen bonds are the 'chemical glue' that binds two molecules together and makes them act as one. They are crucial in applications such as enzyme kinetics, DNA replication and the binding of drugs to specific targets in the body.



Project lead: Janet E. Del Bene, Ph.D., Youngstown State University
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New material could improve efficiency of solar power

Ohio State University chemists and their colleagues have created a new material that overcomes two of the major obstacles to solar power: it has an absorption spectrum that closely matches that of the solar spectrum, and it generates long-lived excited electrons that should allow solar cells to generate electricity more efficiently.

To design the hybrid material, which combines electrically conducive plastic with metals, including molybdenum and tungsten, the chemists first explored different molecular configurations using the high performance computing systems at the Ohio Supercomputer Center. Then, with colleagues at National Taiwan University, they synthesized molecules of the new material in a liquid solution, measured the frequencies of light the molecules absorbed, and also measured the length of time that excited electrons remained free in the molecules.

The chemists found that the new hybrid material emits photons in two different energy states — one called a singlet state, and the other a triplet state. While both energy states are useful for solar cell applications, the triplet state lasts much longer than the singlet state — which improves the ability to harness their power, explained Malcolm Chisholm, Ph.D., distinguished university professor and chair of the department of chemistry at Ohio State.

At this point, the material is years from commercial development, but Dr. Chisholm added that this experiment provides a proof of concept — that hybrid solar cell materials can offer unusual and beneficial properties. ■

Project lead: Malcolm Chisholm, Ph.D., The Ohio State University
Research title: The remarkable influence of MM delta orbitals with oligothiophenes
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