



Quantum Chemistry Aids the Design of Bio-Inspired Drugs and Materials

Project Purpose: *To use quantum chemistry to model the influence of fluorine atoms on the structure of organic compounds.*

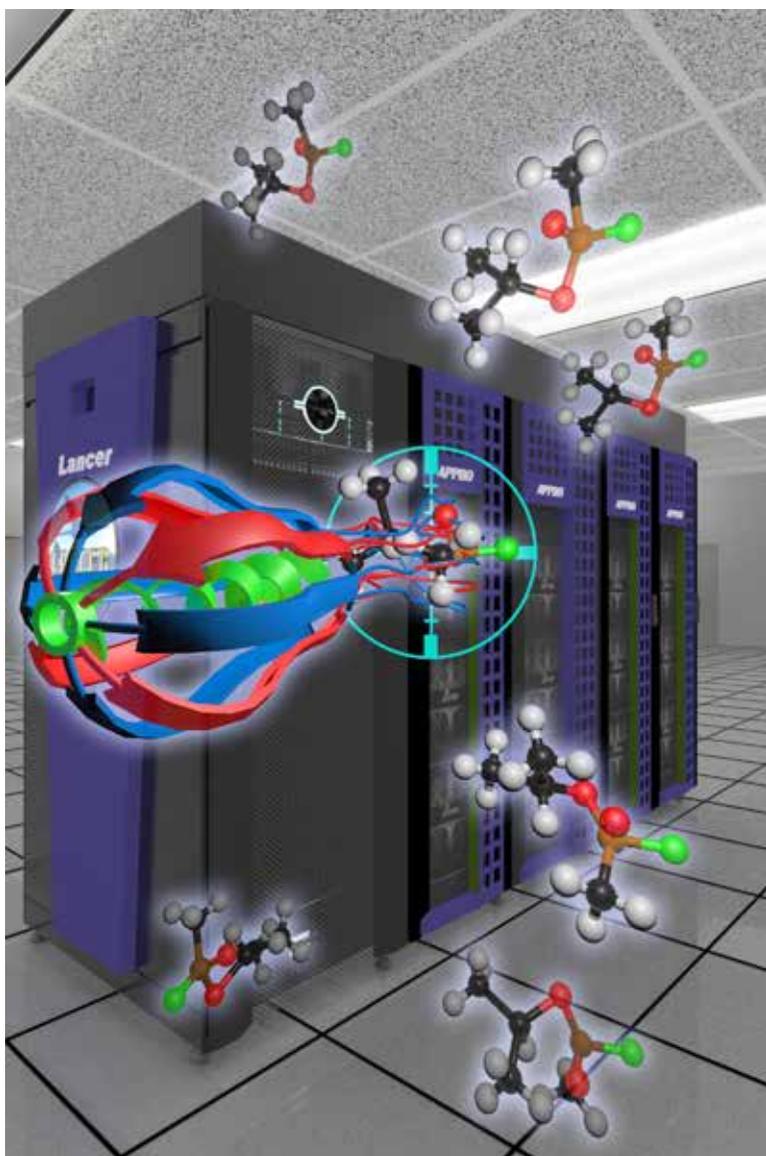
Lancer, a Nanotech Workbench:

Dr. Gary Kedziora, a PETTT (Productivity Enhancement, Technology, Transfer and Training), researcher at the ARFL DSRC, is studying the structure and relative energies of cyclic organic molecules designed to study the influence of fluorine atoms on the structure of biological molecules. Using one of AFRL's newest high-performance computers called LANCER, Dr. Kedziora is successfully modeling the effects of fluorine atoms attached to these cyclic molecules in an effort to better understand how fluorine substitution affects their structure.

Dr. Kedziora's research on LANCER is forming the foundation for other scientists to gain a better grasp of how to modify protein structure and is thereby helping to nurture the design of future bio-materials. "We currently can help experimentalists understand the structures of molecules and how that structure is related to properties" says Dr. Kedziora. "We are entering into an age where we're building the knowledge, the codes, and the machinery to start computationally designing materials. The eventual goal is to modify biological molecules with fluorine so that it has desired properties."

IMPACTS:

- *Paves the way for new drugs and biological materials*
- *Establishes a calculated standard for the preferred structures in certain molecules*
- *Provides insight into how fluorine changes the structure of molecules*
- *Provides a basis for understanding how to modify drugs and peptides with fluorine to engineer their structure*



Apsi-loop motif representation of a hypothetical engineered protein is superimposed on HPC system LANCER, along with sarin molecules, a colorless, odorless liquid, used as a chemical weapon.

Dr. Gary Kedziora, a PETTT Computational Chemistry and Materials researcher working with U.S. Naval Academy Professor Joe Urban, successfully ran a large GAMESS job on Lancer, the shared memory test system. The job used 128 cores and 333 GB of memory.