



2013-14

Hirschfelder Lectures in Theoretical Chemistry

Professor Jack Simons, University of Utah

The Wonderful World of Molecular Anions

Monday, October 7 2:00 p.m. Room 1315 Chemistry

I will briefly review the evolution of the theoretical treatment of molecular anions, and then I will introduce the audience to several families of anions in a way that I expect will produce many interesting surprises. Connections will be made to experiments that probe the characteristics of the anions I will discuss. My hope in this seminar, which is aimed at a broad chemistry audience, is to illustrate how anions display behavior that is challenging to understand yet fun to explore.

How low-energy electrons can damage DNA or repair damage within DNA

Tuesday, October 8 11:00 a.m. Room 1315 Chemistry

I will discuss our efforts to understand and explain how low-energy electrons (e.g., having kinetic energies even below 20 kcal mol^{-1}) can induce covalent bond cleavages in DNA and our predictions as to which bonds are broken when such strand breaks occur. I will also describe our theoretical efforts to explain how photo-excitation of proximal modified guanine residues can repair thymine-dimer damage sites in DNA and our suggestions for designing even better repair agents.

How electrons attach to peptides in ETD/ECD mass spectrometry experiments to generate very specific bond cleavages and fragment ions

Wednesday, October 9 2:00 p.m. Room 1315 Chemistry

I will describe our theoretical efforts to explain how electrons (either free electrons as in electron-capture dissociation or electrons transferred from an anionic reagent as in electron-transfer dissociation) attach to multiply positively charged polypeptides and induce N-C_α bond cleavages along the peptide's backbone. The discussion will deal with Rydberg orbitals and intramolecular electron transfer theory. This subject is related to pioneering work carried out in the Coon laboratory at Wisconsin, so it should be of interest to analytical as well as physical and theoretical chemists.