



OSA and Department of Chemistry Present:

Prof. Benjamin Schwartz

UCLA

“Ultrafast Studies of Charge Transfer Between Atoms in Liquids: The Breakdown of Linear Response”

WHEN: Friday, Oct 12, 2007, 2:00 - 3:00 PM
WHERE: 2201 Natural Sciences 2

(Refreshments will be provided)

Abstract

Molecular liquids differ from each other not only in their ability to make or accept hydrogen bonds and their polarity but also in their intrinsic packing. We have found that the way a solvent packs can have a dramatic effect on the dynamics of electron transfer reactions. Using a combination of nonadiabatic mixed quantum/classical molecular dynamics simulations and ultrafast pump-probe spectroscopy, we show that a highly unusual packing motif in liquid THF makes charge transfer dynamics in this solvent quite different from those in other solvent such as water. We find that even far from its critical point, liquid THF is naturally full of holes that have the right polarity and solvent structure to easily trap an excess electron; the presence of these holes has important implications for charge-transfer-to-solvent (CTTS) dynamics. We also find that the way in which weakly polar solvents such as THF distribute counterions around a reacting solute can dramatically alter not only the rate but even the products of a photoinduced charge transfer reaction; for example, we have directly observed the photoinduced transfer of an electron from an iodide ion to its sodium counterion in liquid THF. Finally, we have been able to prepare neutral Na atoms in THF as the product of two different electron transfer reactions; the results indicate that the linear response approximation, which is intrinsic to most theories of electron transfer, fails even for the relatively simple case of atomic charge transfer reactions.*

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