PHYSICAL CHEMISTRY SEMINAR



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"Understanding Unconventional Doping Mechanisms in Organic Semiconductors"

Abstract: The ability to precisely control the equilibrium carrier concentration in organic semiconducting devices is of great interest. As early as 1977, it was shown that the conductivity of polyacetylene could be systematically controlled over 11 orders of magnitude by doping using a range of halogens. The conventional picture of doping organic semiconductors involves full electron transfer from the semiconductor to the dopant (p-doping) or from the dopant to the semiconductor (n-doping) and the formation of species (polarons or bipolarons) that are the itinerant charge carriers. This process is known as "molecular doping", which requires matching of the energy levels between the semiconductor and the dopant. Unconventional doping methods that do not require energy level matching are desirable; however, mechanistic details of these doping processes remain poorly understood. In this talk, I will discuss tuning the conductivity of conjugated polymers containing Lewis basic sites by Lewis acids. Addition of the Lewis acid effectively p-dopes the hole transport in the parent polymer, leading to increases in the free hole density and conductivity. This methodology is advantageous since the polymer and Lewis acid have excellent solubility in organic solvents, negating the need for co-solvents that uses in molecular dopant such as F₄TCNQ. We use a combination of techniques including electrical measurements, optical absorption, XPS, UPS, IPES, and electron paramagnetic resonance (EPR), electron-nuclear double resonance (ENDOR), nuclear magnetic resonance (NMR), and gas chromatography techniques in conjunction with density functional theory, to gain insight into the doping mechanism by Lewis acids and to explain why the doping efficiency is much higher in the case of Lewis acids as compared to F₄TCNQ.