

**Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING**

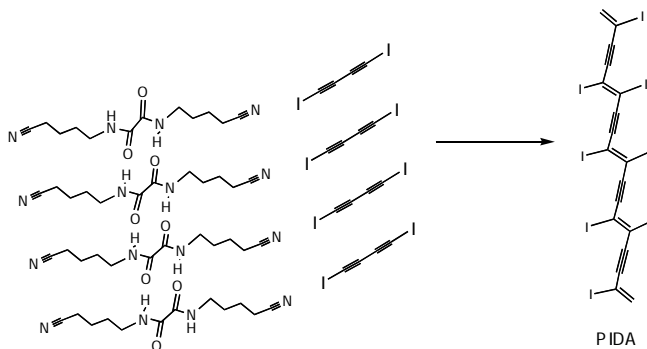
April 8th, 2011, 3:00 pm – SP-S110

***Halogen Bonding: Exploiting a Non-Covalent Interaction
to Make New Materials***

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Iodoalkynes are useful synthons for all-carbon and carbon-rich materials. The Lewis acidity of the iodine atoms in these compounds makes them excellent partners in "halogen bonds" with Lewis bases such as amines and nitriles. These halogen bonds lead to surprising solvent effects on the ¹³C NMR of iodoalkynes, which can be modeled and explained by *ab initio* calculations. Based on such halogen bonds, Lewis-basic co-crystallizing agents, such as bis(pyridyl) or bis(nitrile) oxalamides, can for example be used to control the assembly of diiodobutadiyne (C4I2) in the solid state, leading to crystal packings in which the diyne monomers are well aligned for solid-state polymerization. From such co-crystals, the Goroff group has prepared the novel conjugated polymer poly(diiododiacetylene), or PIDA, the first polydiacetylene with only single-atom side groups. Further studies suggest that the iodine atoms of PIDA are themselves both Lewis acidic and quite labile, making PIDA a promising precursor to carbon-only materials, including the one-dimensional carbon allotrope.



Nancy Goroff is an Associate Professor in the Department of Chemistry at the State University of New York at Stony Brook. She received a Ph.D. degree in organic chemistry in 1994 from the University of California, Los Angeles. There, she worked under Prof. François Diederich on the chemistry of all-carbon and carbon-rich molecules. Following her Ph.D., she obtained a National Science Foundation postdoctoral fellowship and worked under Prof. James Jackson at Michigan State University, where she synthesized and investigated the reactivity and properties of sterically hindered alkynyl carbenes, from which she obtained a patent in 1993 on a one-step air oxidation reaction of cyclohexane to produce adipic acid. She then worked as a Research Corporation postdoctoral fellow under Prof. Brian Coppola and Prof. Seyhan Ege, at the University of Michigan, in their nationally recognized curriculum-development program in chemical education. She was hired as Assistant Professor at the State University of New York in 1997 and she received a National Science Foundation CAREER Award in 2000. Her research interests focus on finding new conjugated molecules with unusual electronic and optical properties. The research involves organic synthesis and standard characterization techniques, including computer modeling and low-temperature spectroscopy.

