

SPECIAL PHYSICAL CHEMISTRY SEMINAR

Thursday
October 17, 2013

3:30 pm

Room 1315
Chemistry

NMR and SAXS Analysis of Complex Materials: Nanodiamond, Bone, and the Nafion Fuel Cell Membrane



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Host: Silvia Cavagnero

Advanced solid-state nuclear magnetic resonance (NMR) techniques, complemented by small-angle scattering analysis, have been used to elucidate the structure and dynamics of complex organic materials and nanocomposites with interesting properties, such as carbon materials, nanodiamond, bone, and the Nafion fuel-cell membrane. The chemical structure is analyzed by combining spectral editing and 2D ^{13}C NMR spectroscopy, while the proximity of functional groups on the nanometer scale is probed using the distance-dependent dipolar couplings between nuclear spins. In addition, the shape of nanostructures is determined by quantitative simulations of small-angle scattering curves using multidimensional Fourier transformation. Our detailed characterization of carbon materials made by low-temperature pyrolysis and of nanodiamond shows them to exhibit opposite extremes of aromaticity. In bone, we discovered that the calcium phosphate nanocrystals that provide this nanocomposite with stiffness are studded with strongly bound citrate, which stabilizes the thin nanocrystals. The hydrated Nafion ionomer used in proton exchange membranes of H_2/O_2 fuel cells contains long, parallel water channels of ~ 2.5 nm diameter, according to our quantitative SAXS simulations that has ruled out a dozen other models. The channels are stabilized by the hydrophilic side groups and the considerable rigidity of the Nafion backbones confirmed by NMR, and can explain important properties of Nafion, including fast diffusion of water and protons.

Refreshments will be available prior to the seminar at 3:15 pm outside room 1315