



CHEMISTRY SEMINAR 291

NMR Crystallography: An Atomic-Resolution Probe of Structure, Function, and Mechanism for Materials Science and Structural Biology

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CCB

University of California, Riverside

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ABSTRACT

My group is developing NMR crystallography – the synergistic combination of solid-state NMR, X-ray diffraction, and first-principles computational chemistry – as an atomic-resolution probe of structure and function across the molecular sciences. I will present two examples from our recent work that highlights its development and application. The first connects molecular level structural rearrangement with macroscopic response in the photomechanical expansion of molecular crystal nanorods. The second reveals chemically-rich structure (by which we mean the location of all atoms, including hydrogen) in the enzyme active site of the pyridoxal-5'-phosphate-dependent enzyme tryptophan synthase, and how this has fundamentally changed our understanding of the mechanism and reaction specificity.

BIO:

Len Mueller is Professor of Chemistry at the University of California, Riverside. He received his B.S. in Chemistry from the University of Rochester (1988), C.P.G.S. in Natural Science (Chemistry) from the University of Cambridge (1989), and Ph.D. in Chemistry from the California Institute of Technology (1997). From 1996-1998 he was an American Cancer Society Postdoctoral Fellow at the Massachusetts Institute of Technology. Len's research interests include nuclear magnetic resonance spectroscopy as a probe of molecular and biological structure and dynamics.

