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## Special Guest Lectures

**Constant pH Molecular Dynamics: Gaining Atomic-level Insights into Protonation-related Phenomena****Jana Shen, University of Oklahoma**

Assistant Professor, Department of Chemistry &amp; Biochemistry

Choppin Hall 210

February 25, 2011 - 11:00 am

**Abstract:**

This candidate lecture will focus on Shen's future research. Abstract not available.

**Speaker's Bio:**

Jana Shen is currently an Assistant Professor at the University of Oklahoma's Department of Chemistry & Biochemistry. She received a Diplom. Chemistry from Universitat Wuppertal, Germany (1995); M.Sc in Theoretical Chemistry from University of Calgary, Canada (1999); and a Ph.D. in Physical Chemistry from University of Minnesota (2003). Shen's research focuses on uncovering microscopic details and physical principles that govern protein folding, stability and interactions. More specific, she and her colleagues are further developing the constant pH molecular dynamics technique to enable fully atomistic studies of pH-dependent conformational phenomena and more accurate electrostatic calculations for proteins and nucleic acids; developing both simulation approaches and novel strategies that exploit experimental data to offer residue-specific characterization of protein unfolded states; and developing new theoretical methods and simulation tools that can be used to solve problems of industrial interest.

