Temperature and Pressure effects on folding/unfolding of proteins
ANGEL GARCIA, Department of Physics and Astronomy

High hydrostatic pressures change the energy landscape of proteins, affecting the thermodynamics and kinetics of folding. Proteins denature at high hydrostatic pressures, implying that the unfolded proteins in aqueous solution have lower volume than the folded state. A model that explains pressure unfolding requires water to penetrate the protein interior and disrupt the protein hydrophobic core. I will explore the energetics of water penetration and the effect of pressure on hydrophobic interactions. I will also describe molecular simulations of the reversible folding/unfolding equilibrium as a function of density and temperature of solvated peptides that can form alpha helices (the AK peptide) and beta hairpins (the C terminal domain of protein G). I will characterize the structural, thermodynamic and hydration changes as a function of temperature and pressure. To study protein folding equilibrium thermodynamics we use an extension of the replica exchange molecular dynamics (REMD) method that allows for density and temperature Monte Carlo exchange moves.