University of Texas at San Antonio

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3:15p.m.-4:15p.m.

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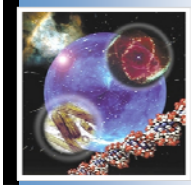
The Inner World of Proteins as Seen by the "Electrostatic Eyes" of Tryptophan

Thousands of scientists studying proteins rely on the intensity and wavelength of emitted light (fluorescence) from the amino acid tryptophan (Trp) because it is extremely sensitive to its "environment" in a protein. This means in practice that most structural changes in a protein during its function will cause a change in fluorescence intensity or wavelength of a strategically placed Trp. Until recently, however, what was meant by "environment" and details of how it controlled fluorescence intensity was not understood. In the last several years, we have combined classical molecular dynamics with simplified quantum mechanics to gain considerable predictive power and insight. This success came from placing more emphasis on the density of states (i.e. resonance and fluctuations) instead of the more commonly emphasized electronic coupling. I will report on how surprising motifs of water dynamics in concert with strong electric fields from protein enter into this microscopic picture of fluorescence behavior. Examples of application will include how Trp fluorescence is able to report the global folding rate of a highly studied protein.



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