Abstract Submitted
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Information theory resolution limits and hidden Markov model analysis of single molecule fluorescence[1] DAVID TALAGA, Rutgers University — Time correlated single photon counting determines luminescence lifetime information on a single molecule level. This paper develops a formalism to allow information-theory analysis of the ability of luminescence lifetime measurements to resolve states in a single molecule. It analyzes experimental losses of information due to instrument response, digitization, and background. This paper shows how to use the information theoretical formalism to evaluate the number of photons required to distinguish dyes that differ only by lifetime, by electron transfer quenching, or by FRET. It shows how the differences between the lifetime of signal and background can help distinguish the dye position in an excitation beam. Many systems follow phenomenological kinetics where discrete states are connected by rate equations. However systems with low energetic barriers and multiple interchanging structures are not as amenable to this approach. Such continuous state spaces are best described by Langevin dynamics (LD) and an appropriate Fokker-Planck equation (FPE). This paper develops hidden Markov models (HMMs) for LD and the FPE. It shows how molecular friction and activation barrier along an effective coordinate can be estimated. It utilizes the models to guide the design of single molecule experiments.

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