

Supporting Information

Linking On-State Memory and Distributed Kinetics in Single Nanocrystal Blinking

*Amy A. Cordones, Kenneth L. Knappenberger, Jr.¹, and Stephen R. Leone**

Departments of Chemistry and Physics, University of California and Lawrence Berkeley National Laboratory, Berkeley, California 94720

¹Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida, 32306-4390

Implementation of Multiple Recombination Centers blinking mechanism

In this work a diffusion-based blinking mechanism is simulated using the Multiple Recombination Centers Mechanism. Here we present the exact rate equations and variables used, as taken from References 17 and 21 of the main text. The reader is referred to these references for a thorough discussion of the equations and mechanism.

As specified in the text of this work, time-dependent fluctuations of the hole trapping rate (k_{trap}) are the basis of the simulated blinking behavior. At each time step, k_{trap} is evaluated as the sum of the trapping rates of each trapping site in the active conformation,

$$k_{trap}(t) = \sum_{i=1}^N k_i \sigma_i(t)$$

where the total number of trapping sites $N=10$, the trapping rate of a single active hole trapping site $k_i=3.33 \times 10^7 \text{ s}^{-1}$, and σ_i indicates the configuration of each site (1 for active, 0 for inactive).

The current configuration of each trapping site is also evaluated at each time step, based on the activation ($\gamma+$) and deactivation ($\gamma-$) rates of each site. The rate equations are based on the treatment of interactive two-level systems, as presented in references 17 and 21 of the main text,

$$\gamma_{i\pm} = \gamma_i \text{Exp} \left(\pm 0.27 \sum_i^N (\sigma_i - 0.5) \mp 0.13 \right)$$

and for the i^{th} trapping site,

$$\gamma_i = \gamma_1 a^{i-1}$$

where $a=10^{-1/2}$ and γ_1 is the base rate for the slowest trapping site. Because of the interdependence of the activation/deactivation rates of the trapping sites, the entire distribution of $\gamma_i \pm$ values is varied in this work by a systematic increase of γ_1 , thus increasing the speed of the k_{trap} fluctuations.