

Designing matrix models for fluorescence energy transfer between moving donors and acceptors¹

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ABSTRACT A recipe is given for designing theoretical models for donor-acceptor systems in which fluorescence energy transfer and motion takes place simultaneously. This recipe is based on the idea that a system exhibiting both motion and fluorescence energy transfer can be modeled by specifying a number of "states" and the rates of transitions between them. A state in this context is a set of specific coordinates and conditions that describe the system at a certain moment in time. As time goes on, the coordinates and conditions for the system change, and this evolution can be described as a series of transitions from one state to the next. The recipe is applied to a number of example systems in which the donors and/or acceptors undergo either rotational or translational motion. In each example, fluorescence intensities and anisotropies for the donor and acceptor are calculated from solutions of eigensystems. The proposed method allows for analyzing time-resolved fluorescence energy transfer data without restrictive assumptions for motional averaging regimes and the orientation factor. It is shown that the fluorescence quantities depend on the size of the motional step (i.e., on the number of states), only if fluorescence energy transfer occurs. This finding indicates that fluorescence energy transfer studies may reveal whether the dynamics of a system (e.g., a protein) is better described in terms of transitions between a relatively small number of discrete states (jumping) or a large number of dense states (diffusion).