

MODELING OF CONCENTRATION QUENCHING IN TWO-DIMENSIONAL SYSTEMS

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The phenomenon of concentration quenching has been investigated throughout the last century, however, its origin is not fully understood to this day. An example of such occurrence has been observed in chlorophyll solutions: at higher concentrations the relative fluorescence intensity becomes dependent on concentration and starts decreasing [1]. It is important to note that in artificial systems the fluorescence is usually significantly quenched at fluorophore concentrations typical to that of unquenched *in vivo* photosynthetic systems.

In this work, concentration quenching in a two-dimensional system was simulated using approach similar to Ref. [2]. Molecules were scattered in a certain area using a uniform distribution, and different concentrations were obtained by changing the number of them. When two or more molecules were closer to each other than a certain distance (R_{trap}), they formed a trap; excitation, after reaching a trap, could not escape. At the initial time moment, excitation was distributed equally among all non-trap molecules. Time dependence of the total excitation probability was calculated by solving the system of kinetic equations with energy transfer rates between the molecules being proportional to the inverse sixth power of the distance between the molecules, following the Förster level of description. Obtained results are shown in Fig. 1. As expected, we can observe that in larger concentrations quenching is more rapid.

This model was used to fit the experimental data of chlorophylls in monolayers [3], however, it turned out that such a simple model cannot explain the data sufficiently well, and a more sophisticated model will be presented in the conference.

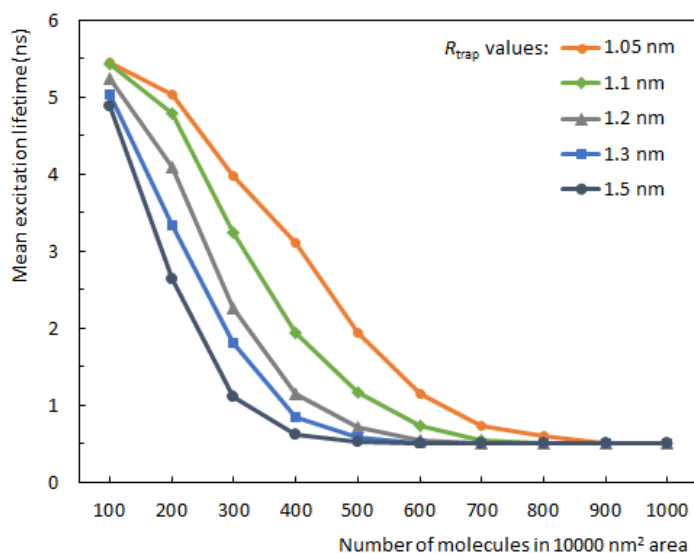


Fig. 1. Dependence of mean excitation lifetime on different molecular concentrations and relative amount of traps.

References

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2. W.-J. Shi, J. Barber, Y. Zhao, *The Journal of Physical Chemistry B* **117** (15), 3976–3982 (2013).
3. M. L. Agrawal, J.-P. Chauvet, L.K. Patterson, *The Journal of Physical Chemistry* **89** (14), 2979–2982 (1985).