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2D electronic spectroscopy - From basics to coherence phenomena in biology

From a quantum mechanical perspective, most molecular systems can be reduced to certain simple discrete level structures. Many properties of such multilevel systems do not depend on their exact nature, e. g. vibrational or electronic. While reflecting distinctly different physics, one common feature is the possibility to excite a coherent superposition of energy eigenstates, referred to as a wavepacket. As shown in numerous recent studies on natural light harvesting complexes, [1] two-dimensional electronic spectroscopy (2D-ES) has a unique disposition for the study of such coherences due to its ability to resolve cross peaks. After a brief introduction of 2D-ES and its experimental implementation, I will present experimental studies on monomers [2] and molecular J-aggregates, [3] where vibrational and vibronic modulations will be discussed. I will present oscillatory features in coupled molecular aggregates involving both electronic and nuclear degrees of freedom. A theoretical model of a vibronic dimer with dissipative dynamics described within Redfield theory succesfully reproduces 90° phase shifts found in recent experimental works. A general conclusion is that a general distinguishing criterion based on the experimental data alone cannot be devised.
[1] Schlau-Cohen, G. S.; Ishizaki, A.; Fleming, G. R. Chem Phys 2011, 386, 1. [2] Mancal, T.; Christensson, N.; Lukes, V.; Milota, F.; Bixner, O.; Kauffmann, H. F.; Hauer, J. J. Phys. Chem. Lett. 2012, 3, 1497. [3] F. Milota, V. I. Prokhorenko, T. Mancal, H. von Berlepsch, O. Bixner, H. F. Kauffmann, and J. Hauer, J. Phys. Chem. A, 10.1021/jp3119605 (2013).

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