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Theoretical evaluation of the nonlinear optical properties of extended π-conjugated chromophores

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Abstract: π-conjugated chromophores with large two-photon absorption (TPA) cross-section are of interest for nonlinear optical (NLO) applications in photonic or electro-optic devices, for instance for optical signal processing, 3D nanofabrications, data storage, or biosensing in cellular environments. To design new chromophores with large TPA cross-sections, it is essential to characterize their electronic and nonlinearoptical properties. We will seek to optimize donor-acceptor chromophores for linear and nonlinear optical response properties. Our computational work seeks to establish structure - NLO properties relationships and to design chromophores with enhanced second-order and/or third-order response using quantum chemical modeling.
References:
1. "A new class of cyanine dyes with large bond-length alternation," S. Ohira, J. M. Hales, K. J. Thorley, H. L. Anderson, J. W. Perry, and J.-L. Bredas. J. Am. Chem. Soc. 2009, 131, 6099-6101.
2. "Porphyrin dimers: A theoretical understanding of the impact of electronic coupling strength on the two-photon absorption properties," S, Ohira and J.-L. Bredas. J. Mater. Chem. 2009, 19, 7545-7550.

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