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Quadrupolar dyes for NLO applications: solvent-induced symmetry breaking and huge TPA cross-sections in aggregates ANNA PAINELLI, GABRIELE D'AVINO, FRANCESCA TERENZIANI, Parma University — Quadrupolar dyes, where electron donor (D) and acceptor (A) groups are linked by π-conjugated bridges to yield symmetrical structures (D-π-A-π-D or A-π-D-π-A) are intensively studied for TPA applications. In an essential-state model for the solvated dyes, symmetry-broken dipolar solutions are found for either the ground or the one-photon excited state. Dyes are accordingly classified in three different classes, with distinctively different spectroscopic behavior. The model provides useful guidelines for the design of molecules for TPA applications and represents a general frame to understand energy transfer processes in multipolar molecular systems. [1] The same essential state model applies to aggregates of quadrupolar dyes. Relaxing the dipolar approximation for electrostatic intermolecular interactions, bound-biexcitons appear with important spectroscopic consequences. Specifically, the large TPA cross-section of quadrupolar dyes is amplified by orders of magnitude as a result of aggregation. [1] F. Terenziani, A. Painelli, C. Katan, M. Charlot, M. Blanchard-Desce, *J. Am. Chem. Soc.* **2006**.

Anna Painelli
Parma University

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