Quantum Chemical Modeling of Excited States, Predictive Theoretical Studies on Boron Dipyrrin Systems

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Excited state dynamics of various popular chromophores (Figure 1) will be discussed. In all cases the theoretical results will be presented with simple and conceptual molecular orbital analyses. General design principles for i) tuning the excited state properties of fluorescent probes and ii) inter-system crossing (ISC) will be introduced.

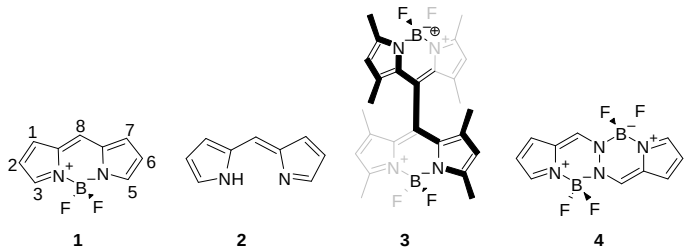

Figure 1. BODIPY (**1**), dipyrrin (**2**), 8,8' orthogonal bis-BODIPY (**3**), and BOPHY (**4**).

Details of excited state electronic structure of BODIPY (**1**) and the contrasting luminescent properties of **1** and dipyrrin (**2**) will be corroborated.[1] A novel and unprecedented feature[2] for a "good" fluorophore with high quantum yield (hence negligible triplet quantum yield), achieved solely by orthogonal dimerization of BODIPYs giving rise to **3** will be introduced. Principles of transforming a fluorophore to an efficient ISC agent (as a promising direction for $^1O_2$ photosensitization in photodynamic therapy (PDT)) will be uncovered.[3] Electronic structure motifs that govern emission, fluorescence quenching and the $S_1 \rightarrow T_1$ transitions will be elaborated. Challenges for designing new fluorophores from scratch will be elaborated by comparing photophysics of **1** and BOPHY (**4**) – the recently discovered cousin of **1**.[4] Our results are promising for understanding and controlling fluorescence action as well as designing new fluorophore cores and intersystem crossers.

References

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