Tracking photoexcitation to sense environment: design of BODIPY-based molecular rotors

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Fluorescent boron-dipyrromethene (BODIPY) derivatives with attached rotating molecular group are known to be sensitive to the viscosity of their immediate surroundings in laboratory solvents [1], polymer solutions [2] and live cells [3]. The challenge is to predict and design the compounds with desired spectroscopic properties without resorting to trial-and-error synthesis.

For this purpose, a potential-energy surface model of the photoexcitation and subsequent fluorescence of the subclass of BODIPY derivatives was developed, backed by time-dependent density functional theory (TD-DFT) computations. It was found that the main feature modulating the viscosity-sensitivity is an energy barrier in the first excited electronic state which separates two local minima. The minima roughly correspond to the emission and non-radiative relaxation pathways which in turn are affected by the properties of the medium.

The current model was applied to explain an increase in sensitivity range [1], to design a red-emitting variant [3] and to guide a potential viscosity or temperature sensor selection based on the height of the energy barrier [4] for different BODIPY derivatives (Fig. 1), while the exact treatment of the polarity dependence remains an open question.

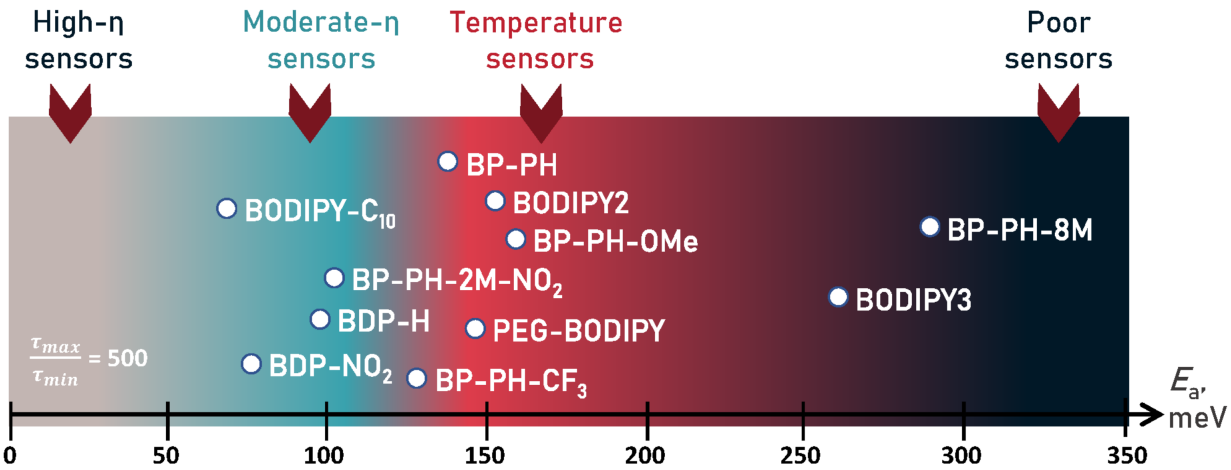

Fig. 1. Sensing potential of BODIPY derivatives based on the height of the energy barrier [4].

REFERENCES

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