Fine-tuning BODIPY molecular sensors by means of computational models

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Boron-dipyrromethene (BODIPY)-based compounds form a class of photoactive molecules whose spectral properties make them promising candidates for use as molecular sensors.[1] However, due to a wide range of possible target environments, purely experimental determination of best-performing derivatives requires many trial-and-error cycles of synthesis and measurement. To aid in the BODIPY sensor design, a quantum chemical model of the photophysical properties of molecules based on BODIPY-phenyl was developed and then used to fine-tune the potential sensors, such as expanding viscosity sensitivity range,[2] shifting the fluorescence wavelength,[3] and aiming to measure either high or moderate viscosity – or temperature.[4]
Still, the initial model was limited to describing non-polar environments. For polar solvents as well as other chemically-dynamic conditions, the models of direct molecular sensor-environment interactions (based on density-functional theory, molecular dynamics and mixed-approach computations) are currently developed. The research includes generalizing over solvents of different polarity,[5] studying experimentally-proposed formation of solvent-solute clusters (Figure 1, left),[6] and investigating sensor self-positioning in lipid bilayer membranes (Figure 1, right).[7]

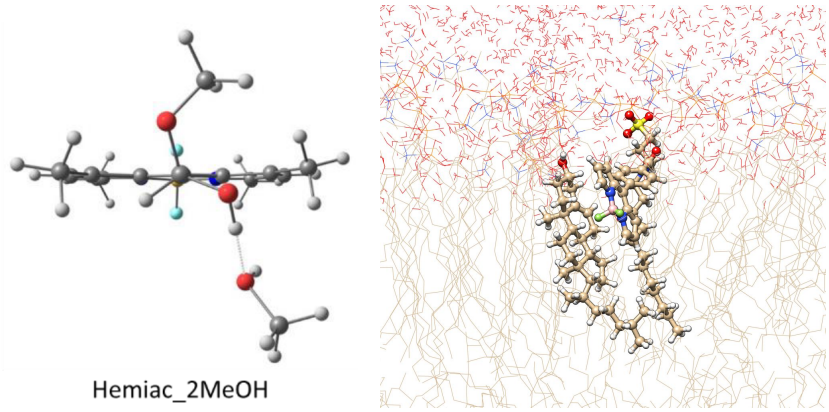

Figure 1: Examples of direct interaction between BODIPY sensor and environment – (left) hemiacetal compound of BODIPY-formyl in methanol, (right) transient compound of specialized BODIPY derivative and cholesterol in a lipid bilayer

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