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# Red to Blue Upconversion Nitric Oxide Sensing and the Localization of Sensors in Liposomes

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Over the past decades, endothelial dysfunction and atherosclerosis have become a significant issue across the world. Nitric oxide (NO), along with calcium, is a primary physiological mediator for detecting endothelial dysfunction as NO plays a crucial role in the proper functioning of endothelial cells. On the other hand, triplet-triplet annihilation upconversion (TTA-UC) has become a powerful tool with promising applications like photocatalysis, solar energy conversion, drug delivery, bio-imaging, and photoactivated chemotherapy. Because of its low energy activation, for example red light, it causes less cell damage and deeper light penetration. Furthermore, in a cellular setting, the anti-stokes wavelength shift during upconversion allows it to be distinguished from the autofluorescence from cells.
Here we will be discussing how we have developed a TTA-UC nitric oxide sensor and the challenges involved in making future TTA-UC sensors. Simulation of the membrane using molecular dynamics calculations to describe the structure of the system is very expensive. Using the novel COSMOplex software, many simulation applications of self-organizing systems are possible at a significantly lower computational cost. This is made possible by using ensembles of thermodynamic states, compared to explicitly modeling the whole system using molecular dynamics. We used the COSMO suite of software to exploit this significantly lower computation costs.
In this communication, we will be discussing the development of our new upconversion nitric oxide sensor capable of sensing nitric oxide in liposome formulation and modeling a simplistic lipid membrane to calculate the relative positions of the different modifications of the sensor in the membrane.

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