Sneak Peek to a Tailor-made Molecular Logic Nitric Oxide Sensor towards Intracellular Diagnostics: A Theoretical Perspective

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Nitric oxide in the endothelium is a critical molecule for regulating vascular function as well as a key predictor of endothelial dysfunction [1] which is notorious for being an important contributor to the progression of atherosclerosis [2], consequently leading to a variety of complications most notably the world's leading cause of death – Coronary Artery Disease (CAD) or Ischemic heart disease as reported by the World Health Organization [3]. Researchers from LOGICLAB (Molecular logic lab-on-a-vesicle for intracellular diagnostics) - Innovative Training Network have designed and synthesized a tailor-made nitric oxide sensing compound for this purpose. In this presentation, we will shed light on the mechanism of this novel Perylene-based logic sensor for the detection of nitric oxide, give insights on ways to enhance its efficiency and tackle its use as an annihilator for triplet–triplet annihilation - upconversion (TTA-UC). Time-dependent density functional theory (TDDFT) methods are employed to decipher the electronic structure of the sensor and the synergy between theory and experiment will be demonstrated.

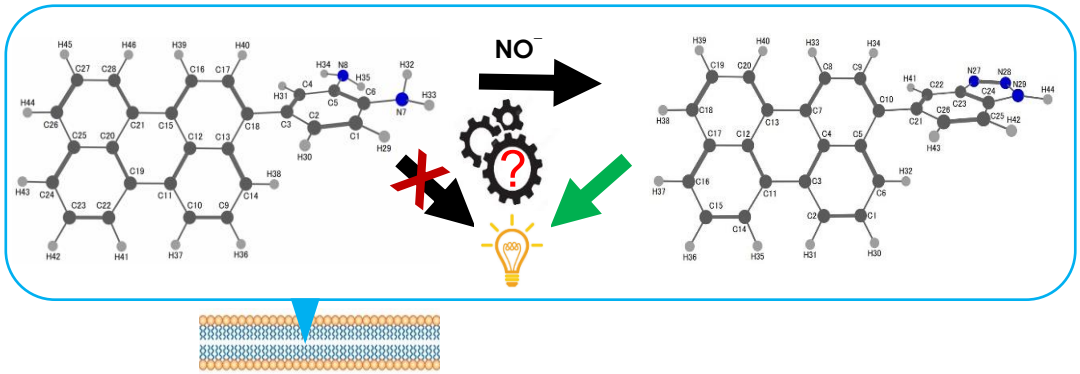

Fig. 1. Surface-level Mechanism of Nitric Oxide Sensing.

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