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Theoretical study of the sensing properties of KL 1421 luminophore interacting with carotenoids

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Applications of sensors vary from measuring temperature to detecting the presence of harmful materials, the variety of sensors occurring due to their advantages in certain situations (for example, non-contact high-precision measurements in harsh environments are performed mostly by optical sensors). In a recent work[1] we demonstrated that the KL 1421 luminophore exhibits selective sensing behavior toward acetic acid vapors, and no significant photoluminescence response was observed for other tested substances.
We further investigated the incorporation of carotenoids in KL 1421 and their effect on its absorption efficiency and sensitivity of the optical sensor[2]. The geometry, its change, and the charge redistribution in KL 1421 when the molecule interacts with carotenoids and/or sensed molecules such as NH_3 and acetic acid, were studied by the B3LYP/cc-pVTZ approach. The increase in molar absorptivity is observed in compounds with carotenoids, leading to higher absorbance of KL 1421. The conjugated double-bond number influences charge redistribution in KL 1421 & carotenoid & sensed molecule compounds. Results of our investigation prove that NH_3 could not be sensed by KL 1421, although this could be possible by KL 1421 & carotenoid, due to the energy level variations and shifts of peaks corresponding to the excitations due to charge transfer from the sensed molecule. Additionally, the singlet-triplet transfer in the compounds with carotenoids is faster than that in KL 1421 & sensed molecule, while the transfer from triple to ground state is longer and more efficient. The molar absorptivity indicates higher absorbance of the compound under study with carotenoids than without them.
In conclusion, carotenoids are good candidates to enhance the sensory properties of KL 1421 novel organic luminophores, opening possibilities for improved sensor applications in biotechnology, nanomaterials and environmental science.

References:

[1]Zabolotnii, V.; Tamuliene, J.; Drava, M. M.; Kirova, T.; Tepliakova, I.; Lukinsone, V.; Kinens, A.; Viter, R. Investigation of structure, optical properties and chemical stability of the pyridinium luminophore with high quantum yield. Applied Materials Today, 2025, 46, 102890-1-102890-11. https://doi.org/10.1016/j.apmt.2025.102890

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