Inversion of the lowest singlet excited states induced by the presence of the silicon atom in a styryl-carbazole derivative

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The main goal of the research was to compare photophysical and spectroscopic properties of the organo silicon compound (styryl-carbazole derivative) with its carbon analogue to point out if there is any significant difference in the emission caused by the presence of the silicon atom. Investigation was performed in solvents of varying polarity. In n-hexane, both the silicon- and the carbon-containing compounds had very similar emission properties. In acetonitrile, the emission properties remained the same for the C-compound but changed significantly for the Si-compound. In particular, the fluorescence spectrum of the latter was red-shifted, and its radiative rate constant was even 7-times larger than in n-hexane which suggested that the emissive state of the silicon-containing compound was different in these two solvents. DFT calculations using the CAM-B3LYP functional showed that the emissive state of the C-compound involves the LUMO+1 orbital regardless of the medium. In contrast, for the Si-compound, changing the medium from n-hexane to acetonitrile resulted in the inversion of the emissive states from an excited state involving the LUMO+1 orbital (the dipole moment $\mu=4.2$ D) to an excited state involving the LUMO orbital ($\mu=8.9$ D). There are known examples in literature showing that silicon can act as a spacer between chromophores or facilitate intramolecular electron transfer. In our research, we reported that introduction of silicon atom affects the emission properties of a styryl-carbazole derivative in changing the order (inversion) of the lowest singlet excited states which results in modification of the emission from ultraviolet to visible spectrum. This effect can be of special interest for light-emitting materials (i.e., light-emitting diodes).

Biography
Karolina Rachuta is a Researcher. She completed her master thesis and then pursuing her research for PhD degree at Adam Mickiewicz University.

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