Quantitative method for determining the effect of the environment on the quantum yield of indole

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Fluorescent chromophores have been extensively used as probes to obtain microscopic information. A particular case is that of tryptophan, which is present in many proteins and allows for both structural and kinetic qualitative information to be obtained. In this seminar, I will show the design and application of three methodologies based on QM/MM molecular dynamics that allow for the quantitative determination of the fluorescence quantum yield of indole (the chromophore of tryptophan) in different solvents.[1] I will also briefly comment on our electronic structure software based on DFT and accelerated by the use of GPUs[2] called LIO.[3]

References

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[3] Marcolongo, J. P.; Zeida, A.; Semelak, J. A.; Foglia, N. O.; Morzan, U. N.; Estrin, D. A.; González Lebrero, M. C.; Scherlis, D. A. *Frontiers in Chemistry* **2018**, *6*.