
How theoretical simulations can help to a better understanding of firefly bioluminescence ?

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Abstract

The emitting light in fireflies arises from the electronic relaxation of oxyluciferin, an organic compound resulting from the oxidation of the D-luciferin substrate inside an enzyme called luciferase.

In order to theoretically study such systems, the use of quantum mechanical/molecular mechanical (QM/MM) methods is required. Accurate QM level is needed for dealing with electronic transition and charge transfer phenomena. Taking into account the surrounding protein at the MM level is essential in order to understand the color modulation and influence of the enzyme. The presentation will discuss some of the results obtained on the firefly bioluminescent system using the coupling of the programs MOLCAS (CASPT2/CASSCF) or G09 (DFT) and TINKER (AMBER force field).

Examples of how theoretical studies can give complementary insights to the experimental results for the understanding of such complex phenomena will be presented. Fluorescence and bioluminescence phenomena will be compared. Influence of the surrounding environment (notably mutation in the luciferase [1] or different luciferases) or artificial modification of the wild type emitter [2] will be presented.

Isabelle Navizet, Ya-Jun Liu, Nicolas Ferré, Hong-Yao Xiao, Wei-Hai Fang, Roland Lindh, *Color-Tuning Mechanism of Firefly Investigated by Multi-Configurational Perturbation Method J. Am. Chem. Soc.* **132** (2010), 704-712.

Romain Berraud-Pache and Isabelle Navizet, *QM/MM calculations on a newly synthesised oxyluciferin substrate: new insights into the conformational effect, PCCP*, **18** (2016), 27460 – 27467.

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