

## Modelling absorption and emission spectra taking into account the dynamic environment: example of firefly bioluminescent systems and analogues

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The emitting light in fireflies or other bioluminescent species 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 have insight of the mechanism of the light emission, both experimental and theoretical joint studies have been performed. Absorption and fluorescence spectra of the products of the bioluminescence are obtained by a combination of molecular dynamics (MD) followed by calculation of the electronic transitions by hybrid (QM/MM) methods. The emission and absorption spectra are accurately reproduced compared to the experimental ones when the dynamic of the system is taking into account.

I will present briefly the used methodology and examples of theoretical studies that can give complementary insights to the experimental results.

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