Research Doctorate (Ph.D.) in Chemical Sciences
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Project Information

1 -Title

Development of theoretical-computational methods for the study and the design of photodynamic therapy agents

2 - Key words

ab-initio molecular dynamics; photochemistry; photodynamic therapy

3 - Abstract

Photodynamic therapy is a promising treatment of a variety of cancer tumor types based on the action of a photosensitizer that, upon irradiation, promotes the formation of highly reactive singlet oxygen, leading to the death of malignant cells. To be highly effective, photosensitizers must be characterized by a large intersystem crossing rate, low dark toxicity, and a singlet− triplet gap close to that of oxygen. The understanding of the photodynamic mechanism and the design of new effective photodynamic therapy agents can greatly benefit from an 'in silico' design, namely a theoretical computational approach capable to disentangle at molecular level the key structural and dynamical features affecting the performance of the photosensitizer.

The present project is aimed at the development of a new computational protocol to study and to design photodynamic therapy agents. The new method will be based on non-adiabatic molecular dynamics in condensed phase, and on a newly developed analysis to recognize the vibrational modes that promote in particular the intercrossing system. As matter of fact, this is the most important feature affecting the singlet oxygen formation quantum yield. The method will be applicated to BODIPYs and polypyrrole macrocyclic photodynamic agents.