

## Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Mercredi 1<sup>er</sup> Juin à 10:30

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## Predicting and interpreting the second-order nonlinear optical responses: from reference molecules to complex systems

This talk will tackle the prediction and the interpretation of the second-order nonlinear optical (NLO) responses by using quantum chemistry approaches. Several aspects will be addressed by going from reference molecules to more complex systems: i) selecting reliable theoretical chemistry methods, ii) the not-straightforward relationships between the measured quantities and the computed ones, iii) the impact of the surrounding (in solution and solid phases), and v) frequency dispersion aspects.

Study cases will include i) reference molecules in gas and liquid phases [1], ii) push-pull  $\pi$ -conjugated systems of various shapes, iii) biological systems [2], iv) molecular switches [3], v) compounds with transition metal atoms, vi) functionalized surfaces [4], vii) organic and hybrid organic-inorganic solids [5]. Several directions for future research and method developments will be sketched.

### References

- (1) F. Castet, E. Bogdan, A. Plaquet, L. Ducasse, B. Champagne, and V. Rodriguez, J. Chem. Phys. 136, 024506 (2012).
- (2) M. de Wergifosse, J. de Ruyck, and B. Champagne, J. Phys. Chem. C 118, 8595-8602 (2014).
- (3) F. Bondu, J. Quertinmont, J.L. Pozzo, V. Rodriguez, A. Plaquet, B. Champagne, and F. Castet, Chem. Eur. J. 21, 18749-18757 (2015).
- (4) S. Nénon and B. Champagne, J. Phys. Chem. Lett. 5, 149-153 (2014).
- (5) T. Seidler and B. Champagne, J. Phys. Chem. C 120, 6741-6749 (2016).

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