Vincent Liegeois
Technological Platform High Performance Computing
Namur Institute of Structured Matter
Namur Institute for Complex Systems
Unit of theoretical and structural physico-chemistry
Namur Institute of Structured Matter

Qualifications

Doctor of Science, Elaboration of quantum chemistry methods for predicting and interpreting vibrational Raman optical activity: applications to helical structures, University of Namur
Award Date: 19 Jun 2008

Research output

1. Colleu T, Fekete A, Gonze X, Cloots A, Liégeois V, Rignanese GM et al. **Surface enhanced infrared absorption mechanism and modification of the plasmonic response**. JPhys Photonics. 2024 Apr;6(2):025003. doi: 10.1088/2515-7647/ad2529
2. D'haese LCG, Daugey N, Pitrat D, Brotin T, Kapitán J, Liégeois V. **Understanding the surrounding effects on Raman optical activity signatures of a chiral cage system: Cryptophane-PP-111**. Spectrochimica Acta. Part A: Molecular and Biomolecular Spectroscopy. 2024 Feb 5;306:123484. doi: 10.1016/j.saa.2023.123484
3. Hood BR, de Coene Y, Torre Do Vale Froes AV, Jones CF, Beaujean P, Liégeois V et al. **Electrochemically-Switched 2nd Order Non-Linear Optical Response in an Arylimido-Polyoxometalate with High Contrast and Cyclability**. Angewandte Chemie. International edition. 2023 Jan 26;62(5):e202215537. doi: 10.1002/anie.202215537
4. Adjieufack AI, Champagne B, Liégeois V. **Investigating the Mechanism of the Catalytic Intramolecular Aza-Wittig Reaction Involved in the Synthesis of 2-Methylbenzothiazole from the Perspective of Bonding Evolution Theory**. Synthesis. 2022 Nov 15;55(13):2070-2082. doi: 10.1055/a-2022-2206
5. Adjieufack AI, Liégeois V, Ndassa Mbouombouo I, Domingo LR, Champagne B. **Unveiling the [3+2] cycloaddition between difluoromethyl diazomethane and 3-ylideneoxindole from the perspective of molecular electron density theory**. New Journal of Chemistry. 2022 Sept 5;46(39):18652-18663. doi: 10.1039/d2nj02685f
6. Zutterman F, Liégeois V, Champagne B. **TDDFT Investigation of the Raman and Resonant Raman Spectra of Fluorescent Protein Chromophore Models**. The Journal of Physical Chemistry. B, Condensed matter, materials, surfaces, interfaces & biophysical. 2022 May 12;126(18):3414-3424. doi: 10.1021/acs.jpcb.2c01202
7. Cecchet F, Liégeois V. **Namur Institute of Structured Matter - NISM: an expert in the synthesis and the characterization of molecular systems and nanostructured materials**. Belgian Research in Europe. 2022;2022.
8. Sharma N, Maciejczyk M, Hall D, Li W, Liégeois V, Beljonne D et al. **Spiro-Based Thermally Activated Delayed Fluorescence Emitters with Reduced Nonradiative Decay for High-Quantum-Efficiency, Low-Roll-Off, Organic Light-Emitting Diodes**. ACS Applied Materials & Interfaces. 2021 Sept 22;13(37):44628-44640. doi: 10.1021/acsami.1c12234
9. Adjieufack AI, Liégeois V, Mbouombouo Ndassa I, Champagne B. **Topological investigation of the reaction mechanism of glycerol carbonate decomposition by bond evolution theory**. RSC Advances. 2021 Mar 9;11(17):10083-10093. doi: 10.1039/d0ra09755a
10. Cherni E, Adjieufack AI, Champagne B, Abderrabba M, Ayadi S, Liégeois V. **Density Functional Theory Investigation of the Binding of ThioTEPA to Purine Bases: Thermodynamics and Bond Evolution Theory Analysis**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2020 May 21;124(20):4068-4080. doi: 10.1021/acs.jpca.0c01792
11. Tetsassi Feugmo CG, Liégeois V, Caudano Y, Cecchet F, Champagne B. **Probing alkylsilane molecular structure on amorphous silica surfaces by sum frequency generation vibrational spectroscopy: First-principles calculations**. The Journal of chemical physics. 2019 Feb 21;150(7):074703. doi: 10.1063/1.5080007
12. Cherni E, Champagne B, Ayadi S, Liégeois V. **Magnetically-induced current density investigation in carbohelicenes and azahelicenes**. PCCP : Physical Chemistry Chemical Physics. 2019 Jan 1;21(27):14678-14691. doi: 10.1039/c9cp02071c
13. Adjieufack AI, Liégeois V, Mbouombouo Ndassa I, Ketcha Mbadcam J, Champagne B. **Intramolecular [3 + 2] Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET)**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2018 Sept 20;122(37):7472-7481. doi: 10.1021/acs.jpca.8b06711

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15. Louant O, Champagne B, Liégeois V. **Investigation of the Electronic Excited-State Equilibrium Geometries of Three Molecules Undergoing ESIPT: A RI-CC2 and TDDFT Study**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2018 Feb 1;122(4):972-984. DOI: 10.1021/acs.jpca.7b10881. Epub 2017 Dec 14. doi: 10.1021/acs.jpca.7b10881
16. Champagne B, Beaujean P, De Wergifosse M, Hidalgo Cardenuto M, Liégeois V, Castet F. **Quantum Chemical Methods for Predicting and Interpreting Second-Order Nonlinear Optical Properties: from Small to Extended π-Conjugated Molecules**. In Wojcik M, Nakatsuji H, Kirtman B, Ozaki Y, editors, Frontiers in Quantum Chemistry. Singapore: Springer. 2018. p. 117-138. (Frontiers in Quantum Chemistry). doi: 10.1007/978-981-10-5651-2_6
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19. Louant O, Liégeois V, Verbiest T, Persoons A, Champagne B. **Faraday Effect in Stacks of Aromatic Molecules**. Journal of Physical Chemistry C: Nanomaterials and interfaces. 2017 Jul 5;121(28):15348-15352. doi: 10.1021/acs.jpcc.7b04177
20. Zutterman F, Liégeois V, Champagne B. **Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models**. ChemPhotoChem. 2017 Jun 1;1(6):281-296. doi: 10.1002/cptc.201700002
21. Rauhalahti M, Taubert S, Sundholm D, Liégeois V. **Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials**. PCCP : Physical Chemistry Chemical Physics. 2017;19(10):7124-7131. doi: 10.1039/c7cp00194k
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23. Tetsassi Feugmo CG, Liégeois V, Champagne B. **Theoretical investigation of vibrational sum-frequency generation signatures of functionalized H-Si(111)**. Journal of Physical Chemistry C: Nanomaterials and interfaces. 2015 Feb 12;119(6):3180-3191. doi: 10.1021/jp5119508
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Prizes

1. **Incentive Award 2012**
   Liegeois, V. (Recipient), Unit of theoretical and structural physico-chemistry

   Details

Awarded date	11 Oct 2012
Granting Organisations	Comité de Gestion du Bulletin des Sociétés Chimiques Belges (C.G.B.-C.B.B.)

Projects

1. **ROA_IC: Investigation of the vibrational signatures of molecules having specific interactions with the solvent such as chiral induction**
   Liegeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems

FRS-FNRS ID	40014193
CPO Number	4-1031-K1 FNRS PDR T.0241.23 S. Vincent
1/01/23 → 31/12/26	
Attachment to an Research Institute in UNAMUR	NISM
Nature of activity type	Research

2. **ROA_env: Investigation of the environment effects on the Raman optical activity signatures of flexible solute molecules**
   D'Haese, L. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
   Liegeois, V. (Supervisor), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
   28/10/22 → 28/10/26

Keywords	vibrational spectroscopies, Raman spectroscopy, Raman Optical Activity (ROA), Quantum Chemistry, Simulations théoriques, density functional theory (DFT)

3. **ROA_env: Investigation of the environment effects on the Raman optical activity signatures of flexible solute molecules**
   D'Haese, L. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Technological Platform High Performance Computing
   Liegeois, V. (Supervisor), Unit of theoretical and structural physico-chemistry, Technological Platform High Performance Computing, Namur Institute of Structured Matter

FRS-FNRS ID	40022042
1/10/23 → 31/12/24	
Attachment to an Research Institute in UNAMUR	NISM
Nature of activity type	Dissertation project, Research

4. **SURFASCOPE: Surface Enhanced Spectroscopy by Second-Principles Calculations**

Vibrational spectroscopies of molecules, materials and nanostructures, with light in the infra-red (IR) and optical (Raman) frequency range, are used in many scientific domains, from basic physics to biomedical applications, because these nondestructive methods have unmatched energy resolution and unique identification capabilities. However their limited spatial resolution and their low cross section are major drawbacks. In the last decades, major progress stemmed from the enhancement of spectroscopic responses when the applied electromagnetic radiation is resonant with a nanostructured plasmonic system, usually a surface or a tip, close to which the vibrating molecule is placed, leading to Surface Enhanced Vibrational Spectroscopies (SEVS). The most popular SEVS are SERS (Surface Enhanced Raman Spectroscopies) and SEIRA (Surface Enhanced IR Absorption).
The simulation of SEVS is a major scientific challenge. While the vibrational response of a system can now be computed with high accuracy by first-principles (1stP) quantum atomistic numerical methods, the calculation of the plasmonic response of a nanostructured system relies mainly on classical parameterized approaches. Indeed, 1stP calculations are very demanding in terms of computational time, which proscribes the accurate simulation of the plasmon resonant response of nanostructures, with typically more than one million active electrons. A unified method is however necessary to tackle unanswered questions related to the interpretation of the experimental data. Various efforts have been devoted recently on second-principles (2ndP) methods, targeting mesoscale systems while keeping 1stP accuracy predictive power. 2ndP approaches aim at finding an effective way to reproduce 1stP data while avoiding the full quantum treatment of the electronic system. For the atomic vibrations, effective atomic potentials integrating out electronic degrees of freedom and accurately describing the 1stP Born-Oppenheimer potential energy surface can be constructed. Low-lying electronic excitations have also been tackled recently. However, the current status of the formalism does not deliver the crucial matching of the dielectric response of the material between the 1stP data and the corresponding 2ndP simulations.
In SURFASCOPE, we will design and implement a 2ndP numerical approach to interpret and guide SEVS. In order to remove the limitations of the existing formalism, the missing density response will be cast in terms of simplified treatments, either non-quantum (e.g. hydrodynamic or atomic polarizability), or quantum (e.g. simplified pseudo-orbitals or localized plasmon-poles). We will interface this 2ndP approach with at least two different state-of-the-art 1stP software packages based on quantum chemistry and material science methods. The effect of the plasmonic local field on the vibrational properties (frequency, activity,...) will then be fully described for systems of millions of electrons with a precision that will be derived from 1stP. This approach will allow us to deal with realistic nanostructured systems. We will demonstrate the capabilities of the new methodology by studying paradigmatic systems, recently investigated experimentally, based on graphene, gold resonant picocavities and metallic nanoantennas.
Gonze, X. (PI), IMCN, UCL
RIGNANESE, G. M. (PI), IMCN, UCL
Henrard, L. (PI), Namur Institute of Structured Matter, Unite de recherche en physique du solide
Liegeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
Colleu, T. (Researcher), Namur Institute of Structured Matter, Unite de recherche en physique du solide
Matatu Mbengo, C. (Researcher), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
1/10/19 → 30/09/24

Attachment to an Research Institute in UNAMUR	NISM
Nature of activity type	Research
Collaborators	IMCN, UCL

5. **Novel Supramolecular Drugs for a “Supramolecular” Disease**

Champagne, B. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
Liegeois, V. (CoI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems
Dory, Y. L. (CoI), Université de Sherbrooke
GENDRON, L. (CoI), Université de Sherbrooke
Ryczko, D. (CoI), Université de Sherbrooke
Soldera, A. (CoI), Université de Sherbrooke

FRS-FNRS ID	34657125

1/09/19 → 31/08/22

Attachment to an Research Institute in UNAMUR	NISM
Nature of activity type	Research
Collaborators	Université de Sherbrooke

6. **Condensed Phase Polarizability: Condensed phase effects on the polarizabilities of organic molecules and ions**
Financement FNRS et PAN (Académie Polonaise des Sciences)
Champagne, B. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems
Liegeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems
Krawczuk, A. (PI), Jagiellonian University
Gryl, M. (PI)
1/06/18 → 31/12/18

Collaborators Jagiellonian University

7. **Elaboration de méthodes de chimie quantique pour prédire et interpreter les spectres vibrationnels de molécules à l'état excité**
LOUANT, O. (PI), Faculty of Sciences
CHAMPAGNE, B. (Supervisor), Unit of theoretical and structural physico-chemistry
Liégeois, V. (Supervisor), Unit of theoretical and structural physico-chemistry
1/10/14 → 30/09/18

8. **Cristaux liquides pour l'optique non-linéaire : conception, synthèse et caractérisation**
Financement Wallonie-Bruxelles International et FRQ-NT
CHAMPAGNE, B. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
Soldera, A. (PI), Université de Sherbrooke
SEIDLER, T. (PI), Unit of theoretical and structural physico-chemistry
TETSASSI FEUGMO, C. G. (PI), Faculty of Sciences, Unit of theoretical and structural physico-chemistry
Liégeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems
1/09/15 → 31/10/17

Collaborators Université de Sherbrooke

9. **Quantum chemical design of open-shell nonlinear optical materials**
FNRS-JSPS
Nakano, M. (PI), Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science
Champagne, B. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
Plaquet, A. (PI)
Liegeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter
DE WERGIFOSSE, M. (PI)
Seidler, T. (PI), Unit of theoretical and structural physico-chemistry
1/01/14 → 31/12/15

Collaborators Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science

10. **Simulation et interprétation des spectroscopies vibrationnelles optiquement actives par les méthodes de la chimie quantique - applications à des structures moléculaires et supramoléculaires chirales.**
Champagne, B. (PI), Unit of theoretical and structural physico-chemistry
Liegeois, V. (PI)
1/10/12 → 30/09/13

11. **Chirality and molecular properties**
Our aim is the development of simulation methods of molecular properties specific to chiral structures in partnership with several experimental groups. Both vibrational signatures and linear and nonlinear optical properties are addressed in these simulations
Champagne, B. (PI), University of Namur
Liégeois, V. (PI), University of Namur
BOTEK, E. (Researcher), University of Namur
Guillaume, M. (Researcher), University of Namur
Quinet, O. (Researcher), University of Namur
1/01/04 → 31/12/12

Keywords theoretical simulations, chirality

12. **Functional Supramolecular Systems (PAI P6/27)**
{description_courte}
Champagne, B. (PI), University of Namur
Wouters, J. (PI), University of Namur
BOTEK, E. (Researcher), University of Namur
DE WERGIFOSSE, M. (Researcher), University of Namur
GUTHMULLER, J. (Researcher), University of Namur
Liegeois, V. (Researcher), University of Namur
NORBERG, B. (Technician), University of Namur
Plaquet, A. (Researcher), University of Namur
STAELENS, N. (Researcher), University of Namur
Vercauteren, D. (CoI), University of Namur
1/01/07 → 31/12/11

13. **Vibrational spectroscopies and theoretical simulations**
Our working aims at developing and implementing quantum chemistry (QC) methods for accurate simulation of spectra based on electric, magnetic, vibrational and mixed phenomena with particular emphasis on Raman optical activity (ROA), circular dichroism (CD), nuclear magnetic resonance (NMR) and sum-frequency generation (SFG) spectroscopies for which experimental aspects will be tackled in parallel.
Champagne, B. (PI), University of Namur
BOTEK, E. (Researcher), University of Namur
Liégeois, V. (Researcher), University of Namur
d'Antuono, P. (Researcher), University of Namur
1/01/07 → 31/12/08

Keywords CD, NMR, spectroscopy, quantum chemistry, SFG, ROA

14. **Elaboration of quantum chemistry methods for simulating the vibrational spectra of chiral structures with inclusion of frequency and electron correlation effects**
Elaboration of quantum chemistry methods for simulating the vibrational spectra of chiral structures with inclusion of frequency and electron correlation effects. These methods will be applied to the characterization of molecular ans supramolecular structures of polymer
Champagne, B. (PI), University of Namur
Liegeois, V. (Researcher), University of Namur
1/10/04 → 1/10/08

Keywords VROA, electron correlation, chirality, Raman, vibrational spectroscopies

15. **COST D26/0010: Experiment-oriented quantum chemistry tools for spectroscopies based on electric, magnetic, and vibrational phenomena**
Our working aims at developing and implementing quantum chemistry (QC) methods for accurate simulation of spectra based on electric, magnetic, vibrational and mixed phenomena with particular emphasis on Raman optical activity (ROA), circular dichroism (CD), nuclear magnetic resonance (NMR) and sum-frequency generation (SFG) spectroscopies for which experimental aspects will be tackled in parallel.
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Keywords CD, NMR, spectroscopy, quantum chemistry, SFG, ROA