

Vincent Liegeois
Namur Institute of Structured Matter
Namur Institute for Complex Systems
Unite de recherche en chimie physique, theorique et structurale
Namur Institute of Structured Matter
Namur Institute of Structured Matter
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Diplômes

Docteur ès sciences, Elaboration of quantum chemistry methods for predicting and interpreting vibrational Raman optical activity: applications to helical structures, Université de Namur
Date d'octroi: 19 juin 2008

Résultats de recherche

1. Kenmogne Tchidjo JF, Adjieufack AI, Chellegui M, Liégeois V, Ndassa IM, Champagne B. **Shedding Light on the Reaction Mechanism of the Catalytic Aza-Wittig Reaction of 2-Methylbenzoxazole: A Bonding Evolution Theory Analysis.** Journal of Physical Organic Chemistry. 2026 mars;39(3):e70065. doi: 10.1002/poc.70065
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3. Cloots A, Collet T, Liégeois V, Rignanese GM, Henrard L, Gonze X. **Surface plasmon polaritons in multilayer jellium systems: Dispersion and spatial description.** Physical review. B. 2025 avr. 15;111(20):205419. doi: 10.1103/physrevb.111.205419
4. Chellegui M, Adjieufack AI, Trabelsi M, Liégeois V, Champagne B. **Unveiling the Reaction Mechanism of Diels-Alder Cycloadditions between 2,5-Dimethylfuran and Ethylene Derivatives Using Topological Tools.** ChemPhysChem. 2025 mars 15;26(6):e202400896. doi: 10.1002/cphc.202400896
5. Chellegui M, Trabelsi M, Champagne B, Liégeois V. **DFT Investigation of the Stereoselectivity of the Lewis-Acid-Catalyzed Diels-Alder Reaction between 2,5-Dimethylfuran and Acrolein.** ACS Omega. 2025 janv. 14;10(1):833-847. doi: 10.1021/acsomega.4c07888
6. Collet T, Fekete A, Gonze X, Cloots A, Liégeois V, Rignanese GM et coll. **Surface enhanced infrared absorption mechanism and modification of the plasmonic response.** JPhys Photonics. 2024 avr.;6(2):025003. doi: 10.1088/2515-7647/ad2529
7. 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 févr. 5;306:123484. doi: 10.1016/j.saa.2023.123484
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9. 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
10. 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
11. 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 mai 12;126(18):3414-3424. doi: 10.1021/acs.jpcc.2c01202
12. 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.
13. Sharma N, Maciejczyk M, Hall D, Li W, Liégeois V, Beljonne D et coll. **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/acsaami.1c12234
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15. 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 mai 21;124(20):4068-4080. doi: 10.1021/acs.jpca.0c01792
16. 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 févr. 21;150(7):074703. doi: 10.1063/1.5080007
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18. 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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21. 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.** Dans Wojcik M, Nakatsuji H, Kirtman B, Ozaki Y, éditeurs, *Frontiers of 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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Prix

1. **Incentive Award 2012**
Liégeois, V. (Bénéficiaire), Unite de recherche en chimie physique, theorique et structurale

Détails

Date de l'octroi	11 oct. 2012
Organisations subventionnaires	Comité de Gestion du Bulletin des Sociétés Chimiques Belges

Projets

1. **ROA_IC: Investigation des signatures vibrationnelles de molécules ayant des interactions spécifiques avec le solvant telles que l'induction de chiralité**
Liégeois, V. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
ID FRS-FRNS 40014193
Numéro de CPO 4-1031-K1 FNRS PDR T.0241.23 S. Vincent
1/01/23 → 31/12/26
Attachement à un institut de recherche NISM reconnu à l'UNAMUR
Nature du type d'activité Recherche
2. **ROA_env: Étude des effets d'environnement sur les signatures d'activité optique Raman de molécules flexibles en solution**
D'Haese, L. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
Liégeois, V. (Promoteur), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
28/10/22 → 28/10/26
mots-clés spectroscopie Raman, spectroscopie vibrationnelle, Chimie Théorique, chimie quantique, théorie de la fonctionnelle de la densité (DFT)

3. **ROA_env: Étude des effets d'environnement sur les signatures vibrationnelles Raman optiquement actives de molécules flexibles en solution**
D'Haese, L. (Responsable du Projet), Namur Institute of Structured Matter, Unite de recherche en chimie physique, theorique et structurale
Liegeois, V. (Promoteur), Unite de recherche en chimie physique, theorique et structurale, Plateforme technologique Calcul intensif, Namur Institute of Structured Matter, Namur Institute for Complex Systems
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1/01/25 → 30/09/26
Attachement à un institut de recherche NISM reconnu à l'UNAMUR
Nature du type d'activité Projet de thèse, Recherche
4. **ROA_env: Étude des effets d'environnement sur les signatures vibrationnelles optiquement actives Raman de molécules flexibles en solution**
D'Haese, L. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter, Plateforme technologique Calcul intensif
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Attachement à un institut de recherche NISM reconnu à l'UNAMUR
Nature du type d'activité Projet de thèse, Recherche

5. 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.

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1/10/19 → 30/09/24

Attachement à un
institut de recherche NISM
reconnus à l'UNAMUR

Nature du type
d'activité Recherche

Collaborateurs IMCN, UCL

6. **Nouveaux Médicaments Supramoléculaires pour une Maladie « Supramoléculaire »**
 Champagne, B. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter
 Liegeois, V. (Co-investigateur), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
 Dory, Y. L. (Co-investigateur), Université de Sherbrooke
 GENDRON, L. (Co-investigateur), Université de Sherbrooke
 Ryczko, D. (Co-investigateur), Université de Sherbrooke
 Soldera, A. (Co-investigateur), Université de Sherbrooke
 ID FRS-FRNS 34657125
 1/09/19 → 31/08/22
 Attachement à un institut de recherche NISM reconnu à l'UNAMUR
 Nature du type d'activité Recherche
 Collaborateurs Université de Sherbrooke
7. **Condensed Phase Polarizability: Condensed phase effects on the polarizabilities of organic molecules and ions**
 Financement FNRS et PAN (Académie Polonaise des Sciences)
 Champagne, B. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
 Liegeois, V. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
 Krawczuk, A. (Responsable du Projet), Jagiellonian University
 Gryl, M. (Responsable du Projet)
 1/06/18 → 31/12/18
 mots-clés Condensed phase, Polarizability, Quantum Chemistry, crystallography
 Collaborateurs Jagiellonian University
8. **Elaboration de méthodes de chimie quantique pour prédire et interpréter les spectres vibrationnels de molécules à l'état excité**
 LOUANT, O. (Responsable du Projet), Faculté des sciences
 CHAMPAGNE, B. (Promoteur), Unité de recherche en chimie physique, théorique et structurale
 Liégeois, V. (Promoteur), Unité de recherche en chimie physique, théorique et structurale
 1/10/14 → 30/09/18
9. **Cristaux liquides pour l'optique non-linéaire : conception, synthèse et caractérisation**
 Financement Wallonie-Bruxelles International et FRQ-NT
 Champagne, B. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter
 Soldera, A. (Responsable du Projet), Université de Sherbrooke
 SEIDLER, T. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale
 TETSASSI FEUGMO, C. G. (Responsable du Projet), Faculté des sciences, Unité de recherche en chimie physique, théorique et structurale
 Liegeois, V. (Responsable du Projet), Unité de recherche en chimie physique, théorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
 1/09/15 → 31/10/17
 mots-clés Cristaux liquides, Optique non linéaire, conception synthèse et caractérisation, Chimie théorique
 Collaborateurs Université de Sherbrooke

10. **Quantum chemical design of open-shell nonlinear optical materials**
 FNRS-JSPS
 Nakano, M. (Responsable du Projet), Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Department of Materials Engineering Science, Osaka Metropolitan University
 Champagne, B. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
 Plaquet, A. (Responsable du Projet)
 Liegeois, V. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
 DE WERGIFOSSE, M. (Responsable du Projet)
 SEIDLER, T. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale
 1/01/14 → 31/12/15
- Collaborateurs Osaka University, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University, Department of Materials Engineering Science, Osaka Metropolitan University
11. **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. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale
 Liegeois, V. (Responsable du Projet)
 1/10/12 → 30/09/13
12. **Chiralité et propriétés moléculaires**
 {description_courte}
 Champagne, B. (Responsable du Projet), Universite de Namur
 Liégeois, V. (Responsable du Projet), Universite de Namur
 BOTEK, E. (Chercheur), Universite de Namur
 Guillaume, M. (Chercheur), Universite de Namur
 Quinet, O. (Chercheur), Universite de Namur
 1/01/04 → 31/12/12
- mots-clés simulations theoriques, chiralité, simulations théoriques, chiralite
13. **Systèmes supramoléculaires fonctionnels (PAI P6/27)**
 {description_courte}
 Champagne, B. (Responsable du Projet), Universite de Namur
 Wouters, J. (Responsable du Projet), Universite de Namur
 BOTEK, E. (Chercheur), Universite de Namur
 DE WERGIFOSSE, M. (Chercheur), Universite de Namur
 GUTHMULLER, J. (Chercheur), Universite de Namur
 Liegeois, V. (Chercheur), Universite de Namur
 NORBERG, B. (Technicien), Universite de Namur
 Plaquet, A. (Chercheur), Universite de Namur
 STAELENS, N. (Chercheur), Universite de Namur
 Vercauteren, D. (Co-investigateur), Universite de Namur
 1/01/07 → 31/12/11
14. **Spectroscopies vibrationnelles et simulations théoriques**
 {description_courte}
 Champagne, B. (Responsable du Projet), Universite de Namur
 BOTEK, E. (Chercheur), Universite de Namur
 Liégeois, V. (Chercheur), Universite de Namur
 d'Antuono, P. (Chercheur), Universite de Namur
 1/01/07 → 31/12/08
- mots-clés CD, spectroscopies, NMR, SFG, ROA, chimie quantique
15. **Elaboration de méthodes de chimie quantique pour la simulation des spectres vibrationnels de structures chirales incluant les effets de la fréquence et de la corrélation électronique**
 {description_courte}
 Champagne, B. (Responsable du Projet), Universite de Namur
 Liegeois, V. (Chercheur), Universite de Namur
 1/10/04 → 1/10/08
- mots-clés corrélation électronique, correlation electronique, VROA, chiralité, spectroscopie vibrationnelle, Raman, chiralite

16. **COST D26/0010: Développement d'outils théoriques et quantiques pour la simulation des spectres basés sur les phénomènes électriques, magnétiques et vibrationnels**

{description_courte}

CHAMPAGNE, B. (Responsable du Projet), Université de Namur

BOTEK, E. (Chercheur), Université de Namur

CAVILLOT, V. (Chercheur), Université de Namur

Guillaume, M. (Chercheur), Université de Namur

Liégeois, V. (Chercheur), Université de Namur

Quinet, O. (Chercheur), Université de Namur

d'Antuono, P. (Chercheur), Université de Namur

1/01/02 → 31/12/06

mots-clés

CD, spectroscopies, NMR, SFG, ROA, chimie quantique