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

Diplômes

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

Résultats de recherche

1. Chellegui M, Trabelsi M, Champagne B, Liegeois 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
2. Colleu 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
3. 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
4. Hood BR, de Coene Y, Torre Do Vale Froes AV, Jones CF, Beaujean P, Liégeois V et coll. **Electrochemically-Switched 2nd Order Non-Linear Optical Response in an Arylimido-Polyoxometalate with High Contrast and Cyclability**. Angewandte Chemie. International edition. 2023 janv. 26;62(5):e202215537. doi: 10.1002/anie.202215537
5. 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
6. 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
7. 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.jpcb.2c01202
8. 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.
9. 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/acsami.1c12234
10. 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 mars 9;11(17):10083-10093. doi: 10.1039/d0ra09755a
11. 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
12. 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
13. Cherni E, Champagne B, Ayadi S, Liégeois V. **Magnetically-induced current density investigation in carbohelicenes and azahelicenes**. PCCP : Physical Chemistry Chemical Physics. 2019 janv. 1;21(27):14678-14691. doi: 10.1039/c9cp02071c

14. 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
15. Nagami T, Fujiyoshi JY, Tonami T, Watanabe KI, Yamane M, Okada K et coll. **Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current**. Chemistry: A European Journal. 2018 sept. 12;24(51):13457-13466. doi: 10.1002/chem.201802696
16. 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 févr. 1;122(4):972-984. DOI: 10.1021/acs.jpca.7b10881. Epub 2017 déc. 14. doi: 10.1021/acs.jpca.7b10881
17. 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 in Quantum Chemistry. Singapore: Springer. 2018. p. 117-138. (Frontiers in Quantum Chemistry). doi: 10.1007/978-981-10-5651-2_6
18. Tetsassi Feugmo CG, Liégeois V, Champagne B. **Coupled-cluster sum-frequency generation nonlinear susceptibilities of methyl (CH3) and methylene (CH2) groups**. PCCP : Physical Chemistry Chemical Physics. 2017 nov. 9;19(44):29822 - 29832. doi: 10.1039/c7cp03509h
19. Fripiat JG, Champagne B, Liégeois V, Harris FE. **Electronic Band Structure of Helical Polyisocyanides**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2017 oct. 19;121(41):7993-8002. DOI: 10.1021/acs.jpca.7b07403. Epub 2017 sept. 13. doi: 10.1021/acs.jpca.7b07403
20. 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 juil. 5;121(28):15348-15352. doi: 10.1021/acs.jpcc.7b04177
21. Zutterman F, Liégeois V, Champagne B. **Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models**. ChemPhotoChem. 2017 juin 1;1(6):281-296. doi: 10.1002/cptc.201700002
22. 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
23. Louant O, Champagne B, Liégeois V. **Numerical differentiation method to calculate molecular properties at ground and excited states - Application to Julolidinemalononitrile**. Chemical Physics Letters. 2015 juin 29;634:249-254. Epub 2015 juin 14. doi: 10.1016/j.cplett.2015.06.014
24. 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 févr. 12;119(6):3180-3191. doi: 10.1021/jp5119508
25. Champagne B, Liégeois V, Zutterman F. **Pigment violet 19-a test case to define a simple method to simulate the vibronic structure of absorption spectra of organic pigments and dyes in solution**. Photochemical and Photobiological Sciences. 2015 févr. 4;14(2):444-456. doi: 10.1039/c4pp00317a
26. Ségerie A, Liégeois V, Champagne B. **Inelastic electron tunneling of C_{60} on gold surfaces from first-principles calculations**. Journal of Physical Chemistry C: Nanomaterials and interfaces. 2015 janv.;119(1):803-818. doi: 10.1021/jp5103093
27. de Wergifosse M, Liégeois V, Champagne B. **Evaluation of the molecular static and dynamic first hyperpolarizabilities**. International Journal of Quantum Chemistry. 2014 juil. 15;114(14):900-910. doi: 10.1002/qua.24685
28. Vanormelingen W, Kesters J, Verstappen P, Drijkoningen J, Kudrjasova J, Koudjina S et coll. **Enhanced open-circuit voltage in polymer solar cells by dithieno[3,2-b:2′,3′-d]pyrrole N-acylation**. Journal of Materials Chemistry A. 2014 mai 28;2(20):7535-7545. doi: 10.1039/c4ta00525b
29. Ségerie A, Lin LL, Liégeois V, Luo Y, Champagne B. **Effects of the basis set and of the exchange-correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol**. Spectrochimica Acta. Part A: Molecular and Biomolecular Spectroscopy. 2014 janv. 1;119:34-41. doi: 10.1016/j.saa.2013.05.025
30. Romanova J, Liégeois V, Champagne B. **Analysis of the resonant raman spectra of viologens and of their radical cations using range-separated hybrid density functionals**. Journal of Physical Chemistry C: Nanomaterials and interfaces. 2014;118(23):12469-12484. doi: 10.1021/jp502318s
31. Romanova J, Liégeois V, Champagne B. **Resonant Raman spectra of molecules with diradical character: Multiconfigurational wavefunction investigation of neutral viologens**. PCCP : Physical Chemistry Chemical Physics. 2014;16(39):21721-31. doi: 10.1039/c4cp02977a
32. Ségerie A, Liégeois V, Champagne B, Lin LL, Luo Y. **Theoretical insight into the inelastic electron tunneling spectra of an anil derivative**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2013 déc. 5;117(48):12783-12795. doi: 10.1021/jp408068d

33. Schwartz E, Liégeois V, Koepf M, Bodis P, Cornelissen JJLM, Brocorens P et coll. **Beta sheets with a twist: The conformation of helical polyisocyanopeptides determined by using vibrational circular dichroism**. Chemistry: A European Journal. 2013 sept. 23;19(39):13168-13174. doi: 10.1002/chem.201300073
34. Feugmo CGT, Liégeois V. **Analyzing the vibrational signatures of thiophenol adsorbed on small gold clusters by DFT calculations**. ChemPhysChem. 2013 juin 3;14(8):1633-1645. doi: 10.1002/cphc.201201077
35. Van Mierloo S, Vasseur K, Van Den Brande N, Boyukbayram AE, Ruttens B, Rodriguez SD et coll. **Functionalized dithienylthiazolo[5, 4-*d*]thiazoles for solution-processable organic field-effect transistors**. ChemPlusChem. 2012 oct. 1;77(10):923-930. doi: 10.1002/cplu.201200132
36. Van Mierloo S, Liégeois V, Kudrjasova J, Botek E, Lutsen L, Champagne B et coll. **Combined experimental-theoretical NMR study on 2,5-bis(5-aryl-3- hexylthiophen-2-yl)-thiazolo[5,4-d]thiazole derivatives for printable electronics**. Magnetic Resonance in Chemistry. 2012 mai 1;50(5):379-387. doi: 10.1002/mrc.3812
37. Tetsassi Feugmo CG, Champagne B, Caudano Y, Cecchet F, Chabal YJ, Liégeois V. **Towards modelling the vibrational signatures of functionalized surfaces: Carboxylic acids on H-Si(111) surfaces**. Journal of physics. Condensed matter. 2012 mars 28;24(12):124111. doi: 10.1088/0953-8984/24/12/124111
38. Liégeois V, Champagne B. **Implementation in the Pyvib2 program of the localized mode method and application to a helicene**. Theoretical Chemistry Accounts. 2012 janv. 1;131(11):1-15. doi: 10.1007/s00214-012-1284-x
39. Liégeois V, Champagne B. **Theoretical investigation of raman optical activity signatures of Tröger's base**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2011 nov. 24;115(46):13706-13713. doi: 10.1021/jp208591j
40. Ségerie A, Castet F, Kanoun MB, Plaquet A, Liégeois V, Champagne B. **Nonlinear optical switching behavior in the solid state: A theoretical investigation on anils**. Chemistry of Materials. 2011 sept. 13;23(17):3993-4001. doi: 10.1021/cm2015516
41. Pelloni S, Carion R, Liégeois V, Lazzeretti P. **The ring current model of the pentaprismane molecule**. Journal of Computational Chemistry. 2011 juin 1;32(8):1599-1611. doi: 10.1002/jcc.21739
42. Drooghaag X, Marchand-Brynaert J, Champagne B, Liégeois V. **Combined experimental and theoretical study on the raman and raman optical activity signatures of pentamethylundecane diastereoisomers**. The Journal of Physical Chemistry. B, Condensed matter, materials, surfaces, interfaces & biophysical. 2010 sept. 16;114(36):11753-11760. doi: 10.1021/jp105028q
43. Liégeois V, Jacob CR, Champagne B, Reiher M. **Analysis of vibrational Raman optical activity signatures of the (TG) and (GG) conformations of isotactic polypropylene chains in terms of localized modes**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2010 juil. 8;114(26):7198-7212. doi: 10.1021/jp102739g
44. Carion R, Liégeois V, Champagne B, Bonifazi D, Pelloni S, Lazzeretti P. **On the aromatic character of 1,2-Dihydro-1,2-azaborine according to magnetic criteria**. Journal of Physical Chemistry Letters. 2010 mai 20;1(10):1563-1568. doi: 10.1021/jz100401y
45. Liégeois V, Jacob CR, Champagne B, Reiher M. **Raman optical activity study of the signatures associated to (TG) and (GG) conformations of isotactic polypropylene chains using mode localization method**. Dans AIP Conference Proceedings. Vol. 1267. American institute of physics. 2010. p. 100-101. (AIP Conference Proceedings). doi: 10.1063/1.3482264
46. Liégeois V. **A vibrational raman optical activity study of 1, 1′ -binaphthyl derivatives**. ChemPhysChem. 2009 août 24;10(12):2017-2025. doi: 10.1002/cphc.200900115
47. Liégeois V, Champagne B. **Vibrational raman optical activity of π-conjugated helical systems: Hexahelicene and heterohelicenes**. Journal of Computational Chemistry. 2009 juin 1;30(8):1261-1278. doi: 10.1002/jcc.21151
48. Champagne B, Guthmuller J, Liegeois V, Quinet O. **Methods for simulating and interpreting vibrational spectra of molecules**. Dans COMPUTATIONAL METHODS IN SCIENCE AND ENGINEERING: Advances in Computational Science. Vol. 1108. American institute of physics. 2009. p. 30-42. (AIP Conference Proceedings). doi: 10.1063/1.3117139
49. Liégeois V, Champagne B. **Analytical Time-Dependent Hartree-Fock Scheme to Evaluate the Vibrational (Hyper)Polarizabilities**. Dans Maroulis G, Theodore E, éditeurs, Computational methods in science and engineering: Advances in computational science. Vol. 1148. American institute of physics. 2009. p. 693-696. (AIP Conference Proceedings).
50. Liégeois V, Champagne B, Lazzeretti P. **Rototranslational sum rules for electromagnetic hypershielding at the nuclei and related atomic Cartesian derivatives of the optical rotatory power**. The Journal of chemical physics. 2008 janv. 1;128(24):244107. doi: 10.1063/1.2943139
51. Liégeois V, Ruud K, Champagne B. **An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra**. The Journal of chemical physics. 2007 nov. 28;127(20):204105. doi: 10.1063/1.2801986
52. Guillaume M, Liégeois V, Champagne B, Zutterman F. **Time-dependent density functional theory investigation of the absorption and emission spectra of a cyanine dye**. Chemical Physics Letters. 2007 sept. 26;446(1-3):165-169. doi: 10.1016/j.cplett.2007.07.105

53. Liégeois V, Quinet O, Champagne B. **Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity**. International Journal of Quantum Chemistry. 2006 déc. 1;106(15):3097-3107. doi: 10.1002/qua.21054

54. Liégeois V, Quinet O, Champagne B, Haesler J, Zuber G, Hug W. **Analysis of the VROA signals of helical heptasilanes using an atomistic approach**. Vibrational Spectroscopy. 2006 nov. 24;42(2):309-316. doi: 10.1016/j.vibspec.2006.05.026

55. Lamparska E, Liégeois V, Quinet O, Champagne B. **Theoretical determination of the vibrational raman optical activity signatures of helical polypropylene chains**. ChemPhysChem. 2006 nov. 13;7(11):2366-2376. doi: 10.1002/cphc.200600451

56. Reiher M, Liégeois V, Ruud K. **Basis set and density functional dependence of vibrational Raman optical activity calculations**. The Journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory. 2005 août 25;109(33):7567-7574. doi: 10.1021/jp052123h

57. Liégeois V, Quinet O, Champagne B. **Vibrational Raman optical activity as a mean for revealing the helicity of oligosilanes: A quantum chemical investigation**. The Journal of chemical physics. 2005 juin 1;122(21). doi: 10.1063/1.1914769

58. Quinet O, Liégeois V, Champagne B. **TDHF evaluation of the dipole-quadrupole polarizability and its geometrical derivatives**. Journal of Chemical Theory and Computation. 2005 avr. 2;1(3):444-452. doi: 10.1021/ct049888y

Prix

1. **Incentive Award 2012**
   Liegeois, 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**
   Liegeois, 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 reconnus à l'UNAMUR	NISM
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
   Liegeois, 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 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
Liegeois, V. (Promoteur), Unite de recherche en chimie physique, theorique et structurale, Plateforme technologique Calcul intensif, Namur Institute of Structured Matter

ID FRS-FRNS	40022042
1/10/23 → 31/12/24	
Attachement à un institut de recherche reconnus à l'UNAMUR	NISM
Nature du type d'activité	Projet de thèse, Recherche

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. (Responsable du Projet), IMCN, UCL
RIGNANESE, G. M. (Responsable du Projet), IMCN, UCL
Henrard, L. (Responsable du Projet), Namur Institute of Structured Matter, Unite de recherche en physique du solide
Liegeois, V. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
Colleu, T. (Chercheur), Namur Institute of Structured Matter, Unite de recherche en physique du solide
Matatu Mbengo, C. (Chercheur), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
1/10/19 → 30/09/24

Attachement à un institut de recherche reconnus à l'UNAMUR	NISM
Nature du type d'activité	Recherche
Collaborateurs	IMCN, UCL

5. **Nouveaux Médicaments Supramoléculaires pour une Maladie « Supramoléculaire »**
Champagne, B. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
Liegeois, V. (Co-investigateur), Unite de recherche en chimie physique, theorique 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 reconnus à l'UNAMUR	NISM
Nature du type d'activité	Recherche
Collaborateurs	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. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter, Namur Institute for Complex Systems
Liegeois, V. (Responsable du Projet), Unite de recherche en chimie physique, theorique 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

7. **Elaboration de méthodes de chimie quantique pour prédire et interpreter les spectres vibrationnels de molécules à l'état excité**
LOUANT, O. (Responsable du Projet), Faculte des sciences
CHAMPAGNE, B. (Promoteur), Unite de recherche en chimie physique, theorique et structurale
Liégeois, V. (Promoteur), Unite de recherche en chimie physique, theorique et structurale
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. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale, Namur Institute of Structured Matter
Soldera, A. (Responsable du Projet), Université de Sherbrooke
SEIDLER, T. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale
TETSASSI FEUGMO, C. G. (Responsable du Projet), Faculte des sciences, Unite de recherche en chimie physique, theorique et structurale
Liégeois, V. (Responsable du Projet), Unite de recherche en chimie physique, theorique 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

9. **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

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. (Responsable du Projet), Unite de recherche en chimie physique, theorique et structurale
Liegeois, V. (Responsable du Projet)
1/10/12 → 30/09/13

11. **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

12. **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

13. **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

14. **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

15. **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), Universite de Namur
BOTEK, E. (Chercheur), Universite de Namur
CAVILLOT, V. (Chercheur), Universite de Namur
Guillaume, M. (Chercheur), Universite de Namur
Liégeois, V. (Chercheur), Universite de Namur
Quinet, O. (Chercheur), Universite de Namur
d'Antuono, P. (Chercheur), Universite de Namur
1/01/02 → 31/12/06

mots-clés CD, spectroscopies, NMR, SFG, ROA, chimie quantique