

Vincent Liegeois
Namur Institute of Structured Matter
Namur Institute for Complex Systems
Unit of theoretical and structural physico-chemistry
Namur Institute of Structured Matter
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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. Liégeois V, Champagne B. **Implementation in the Pyvib2 program of the localized mode method and application to a helicene**. Theoretical Chemistry Accounts. 2012 Jan 1;131(11):1-15. doi: 10.1007/s00214-012-1284-x
2. 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
3. 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 Jul 8;114(26):7198-7212. doi: 10.1021/jp102739g
4. 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**. In AIP Conference Proceedings. Vol. 1267. American institute of physics. 2010. p. 100-101. (AIP Conference Proceedings). doi: 10.1063/1.3482264
5. Liégeois V. **A vibrational raman optical activity study of 1, 1' -binaphthyl derivatives**. ChemPhysChem. 2009 Aug 24;10(12):2017-2025. doi: 10.1002/cphc.200900115
6. Liégeois V, Champagne B. **Vibrational raman optical activity of π -conjugated helical systems: Hexahelicene and heterohelicenes**. Journal of Computational Chemistry. 2009 Jun 1;30(8):1261-1278. doi: 10.1002/jcc.21151
7. Liégeois V, Champagne B. **Analytical Time-Dependent Hartree-Fock Scheme to Evaluate the Vibrational (Hyper)Polarizabilities**. In Maroulis G, Theodore E, editors. Computational methods in science and engineering: Advances in computational science. Vol. 1148. American institute of physics. 2009. p. 693-696. (AIP Conference Proceedings).
8. 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 Jan 1;128(24):244107. doi: 10.1063/1.2943139
9. 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
10. Liégeois V, Quinet O, Champagne B. **Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity**. International Journal of Quantum Chemistry. 2006 Dec 1;106(15):3097-3107. doi: 10.1002/qua.21054
11. 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
12. 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 Jun 1;122(21). doi: 10.1063/1.1914769

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 NISM
UNAMUR

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), Namur Institute of Structured Matter, Unit of theoretical and structural physico-chemistry
Liegeois, V. (Supervisor), Unit of theoretical and structural physico-chemistry, Technological Platform High Performance Computing, Namur Institute of Structured Matter, Namur Institute for Complex Systems

FRS-FNRS ID 40029959
1/01/25 → 30/09/26

Attachment to an
Research Institute in NISM
UNAMUR

Nature of activity type Dissertation project, Research

4. **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 NISM
UNAMUR

Nature of activity type Dissertation project, Research

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.

Gonze, X. (PI), IMCN, UCL

RIGNANESE, G. M. (PI), IMCN, UCL

Henrard, L. (PI), Namur Institute of Structured Matter

Liegeois, V. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter

COLLEU, T. (Researcher), Namur Institute of Structured Matter

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 NISM
UNAMUR

Nature of activity type Research

Collaborators IMCN, UCL

6. **Novel Supramolecular Drugs for a "Supramolecular" Disease**

Champagne, B. (PI), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter

Liegeois, V. (Col), Unit of theoretical and structural physico-chemistry, Namur Institute of Structured Matter, Namur Institute for Complex Systems

Dory, Y. L. (Col), Université de Sherbrooke

GENDRON, L. (Col), Université de Sherbrooke

Ryczko, D. (Col), Université de Sherbrooke

Soldera, A. (Col), Université de Sherbrooke

FRS-FNRS ID 34657125

1/09/19 → 31/08/22

Attachment to an

Research Institute in NISM
UNAMUR

Nature of activity type Research

Collaborators Université de Sherbrooke

13. **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. (Col), University of Namur
1/01/07 → 31/12/11
14. **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
15. **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 and 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
16. **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.
CHAMPAGNE, B. (PI), University of Namur
BOTEK, E. (Researcher), University of Namur
CAVILLOT, V. (Researcher), University of Namur
Guillaume, M. (Researcher), University of Namur
Liégeois, V. (Researcher), University of Namur
Quinet, O. (Researcher), University of Namur
d'Antuono, P. (Researcher), University of Namur
1/01/02 → 31/12/06
- Keywords CD, NMR, spectroscopy, quantum chemistry, SFG, ROA