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Research outputs:

An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets
An extensive analysis has been carried out of the performance of standard families of basis sets with the hierarchy of coupled cluster methods CC2, CCSD, CC3, and CCSDT in computing selected Oxygen, Carbon, and Nitrogen K-edge (vertical) core excitation and ionization energies within a core-valence separated scheme in the molecules water, ammonia, and carbon monoxide. Complete basis set limits for the excitation energies have been estimated via different basis set extrapolation schemes. The importance of scalar relativistic effects has been established within the spin-free exact two-component theory in its one-electron variant (SFX2C-1e).

General information
Publication status: Accepted/In press
Organisations: Department of Chemistry, University of Trieste, Johns Hopkins University, Norwegian University of Science and Technology, Southern Methodist University
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Contributors: Carbone, J. P., Cheng, L., Myhre, R. H., Matthews, D., Koch, H., Coriani, S.
Publication date: 2019

Host publication information
Title of host publication: Advances in Quantum Chemistry
Publisher: Elsevier
(Advances in Quantum Chemistry).
DOIs:
10.1016/bs.aiq.2019.05.005
Source: Scopus
Source ID: 85070683156
Research output: Chapter in Book/Report/Conference proceeding › Book chapter – Annual report year: 2019 › Research › peer-review

Benchmark calculations of K-edge ionization energies for first-row elements using scalar-relativistic core-valence-separated equation-of-motion coupled-cluster methods
Benchmark scalar-relativistic core-valence-separated (CVS) equation-of-motion coupled-cluster ionization potential (EOMIP-CC) calculations of 21 K-edge ionization energies of C, O, N, and F in 14 molecules are reported. The CVS-EOMIP-CC methods are shown to be numerically more stable and more accurate than the parent EOMIP-CC methods, even when the calculations using the latter can be tightly converged. The superior performance of the CVS scheme is attributed to the exclusion of spurious couplings between core-ionized states and valence continuum states. Systematic improvement of computed K-edge ionization energies within the CVS-EOMIP-CC hierarchy, including the CC singles and doubles (CCSD) method, the CC singles, doubles, and triples (CCSDT) method, and the CC singles, doubles, triples, and quadruples (CCSDTQ) method, is demonstrated, with CCSDTQ yielding essentially quantitative results. Maximum absolute deviations between computed and experimental results amount to 2.54 eV for CCSD/cc-pCVQZ, 0.54 eV for CCSDT/cc-pCVQZ, and 0.23 eV for CCSDT/cc-pCVQZ augmented with quadruples contributions using the cc-pVTZ basis sets. The corresponding standard deviations are 1.91 eV for CCSD/cc-pCVQZ, 0.18 eV for CCSDT/cc-pCVQZ, and 0.10 eV for CCSDT/cc-pCVQZ augmented with quadruples contributions using the cc-pVTZ basis sets. Finally, CVS-EOMIP-CCSDT/cc-pCVTZ calculations of core ionization energies in CH$_3$CN and CH$_3$NC are reported, and experimental re-investigation of carbon 1s ionization energies in CH$_3$CN is suggested.

General information
Publication status: Published
Organisations: Department of Chemistry, Johns Hopkins University, Southern Methodist University
Corresponding author: Cheng, L.
Contributors: Liu, J., Matthews, D., Coriani, S., Cheng, L.
Core-valence-separated coupled-cluster-singles-and-doubles complex-polarization-propagator approach to X-ray spectroscopies

The iterative subspace algorithm to solve the complex linear response equation of damped coupled cluster response theory presented, up to CCSD level, by Kauczor et al., J. Chem. Phys., 2013, 139, 211102, and recently extended to the solution of the complex left response multipliers by Faber and Coriani, J. Chem. Theory Comput., 2019, 15, 520, has been modified to include a core-valence separation projection step in the iterative procedure. This allows one to overcome serious convergence issues that specifically manifest themselves at the CCSD level when addressing core-related spectroscopic effects using large basis sets. The spectra, obtained adopting the new scheme for X-ray absorption and circular dichroism, as well as resonant inelastic-X-ray scattering, are presented and discussed. Core-valence separated results for non-resonant X-ray emission are also reported.

Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges

We have investigated the performance of a core-valence separated scheme within the coupled cluster (CC) hierarchy of methods CC singles (CCS), CC singles and approximate doubles (CC2), and CC singles and doubles (CCSD) in reproducing the K-edge x-ray absorption spectra of the low-Z elements carbon, oxygen, and fluorine in formaldehyde (CH₂O), carbonyl fluoride (CF2O), formyl fluoride (CHFO), and formic acid (CHOOH). The analysis covers the entire frequency region from the first 1s → π⁺ excitation to the core-ionization limit, encompassing the region of Rydberg transitions. Moreover, a simulation of the vibronic progressions in the 1s → π⁺ bands of both carbon and oxygen in formaldehyde has been performed at the core-valence separated CCSD level, and the results are critically compared with highly resolved experimental data for this molecule.
Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples

Oxygen, nitrogen, and carbon K-shell photoabsorption and photoionization cross sections have been calculated within core-valence-separated coupled cluster (CC) linear response theory for a number of molecular systems, namely, water, ammonia, ethylene, carbon dioxide, acetaldehyde, furan, and pyrrole. The cross sections below and above the K-edge core ionization thresholds were obtained, on the same footing, from $L^2$ basis set calculations of the discrete electronic pseudospectrum yielded by an asymmetric-Lanczos-based formulation of CC linear response theory at the CC singles and doubles (CCSD) and CC singles and approximate doubles (CC2) levels. An analytic continuation procedure for both discrete and continuum cross sections as well as a Stieltjes imaging procedure for the photoionization cross section were applied and the results critically compared.
New and efficient equation-of-motion coupled-cluster framework for core-excited and core-ionized states

We present a fully analytical implementation of the core-valence separation (CVS) scheme for the equation-of-motion (EOM) coupled-cluster singles and doubles (CCSD) method for calculations of core-level states. Inspired by the CVS idea as originally formulated by Cederbaum, Domcke and Schirmer, pure valence excitations are excluded from the EOM target space and the frozen-core approximation is imposed on the reference-state amplitudes and multipliers. This yields an efficient, robust, practical, and numerically balanced EOM-CCSD framework for calculations of excitation and ionization energies as well as state and transition properties (e.g., spectral intensities, natural transition and Dyson orbitals) from both the ground state and an excited state. The errors in absolute excitation/ionization energies relative to the experimental reference data are of the order of 0.2-3.0 eV, depending on the K-edge considered and on the basis set used, and the shifts are systematic for each edge. Compared to a previously proposed CVS scheme where CVS was applied as a posteriori projection only during the solution of the EOM eigenvalue equations, the new scheme is computationally cheaper. It also achieves better cancellation of errors, yielding similar spectral profiles but with absolute core excitation and ionization energies that are systematically closer to the corresponding experimental data. Among the presented results are calculations of transient-state X-ray absorption spectra, relevant for the interpretation of UV-pump/X-ray probe experiments.

Picosecond timescale tracking of pentacene triplet excitons with chemical sensitivity

Singlet fission is a photophysical process in which an optically excited singlet exciton is converted into two triplet excitons. Singlet fission sensitized solar cells are expected to display a greatly enhanced power conversion efficiency compared to conventional singlejunction cells, but the efficient design of such devices relies on the selection of materials capable of harvesting triplets generated in the fission chromophore. To this aim, the possibility of measuring triplet exciton dynamics with chemical selectivity paves the way for the rational design of complex heterojunctions, with optimized triplet conversion. Here we exploit the chemical sensitivity of X-ray absorption spectroscopy to track triplet exciton dynamics at the picosecond timescale in multilayer films of pentacene, the archetypal singlet fission material. We experimentally identify the signature of the triplet exciton in the Carbon K-edge absorption spectrum and measure its lifetime of about 300 ps. Our results are supported by state-of-the-art ab initio calculations.
Probing local and ultrafast spectroscopies by coupled cluster methods

Resonant Inelastic X-ray Scattering and Nonesonant X-ray Emission Spectra from Coupled-Cluster (Damped) Response Theory
A coupled cluster protocol rooted in damped response theory is presented for computing Resonant Inelastic X-ray Scattering spectra of molecules in gas-phase. Working equations are reported for both linear (i.e., equation-of-motion) and nonlinear parametrizations of the coupled-cluster wave function response. A simple scheme to compute nonresonant X-ray Emission Spectra is also proposed. Illustrative results are presented for water.
Spatial localization in nuclear spin-induced circular dichroism – a quadratic response function analysis

Nuclear magneto-optic (NMO) effects are recently described phenomena originating from the interaction of light with local magnetic fields produced by nuclear spins. The phenomena border nuclear magnetic resonance and optical spectroscopy and are expected to provide rather unique spectroscopic features, borrowing from both localized response of the atomic nuclei as well as more global excitation properties of the whole molecule or its chromophore moieties. A number of quantum-chemical computational studies have been carried out, offering a reasonable agreement with nuclear magneto-optics experiments performed so far. However, the detailed structure-spectra relation is still poorly understood. In this report we address the question of locality of one of the NMO effects, namely nuclear spin-induced circular dichroism (NSCD). We implement an alternative computational approach for calculation of the NSCD intensities, based on residues of quadratic response functions, and use it to investigate the NSCD response of different nuclei in a model molecular system with well-defined separate chromophores. The results show that significant NSCD at a given energy only occurs at the nuclei which are located in the chromophore that is excited. We rationalize these findings using analysis via difference densities, and approximate sum-over-states calculations. This behaviour of NSCD opens a way to experimental studies of localization of excited states in molecules, potentially with resolution down to the order of bond-length.

General information
Publication status: Published
Organisations: Department of Chemistry, University of Oulu
Corresponding author: Štěpánek, P.
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Number of pages: 10
Pages: 18082-18091
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 21
Issue number: 33
ISSN (Print): 1463-9076
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
Original language: English
Electronic versions:
Fulltext
DOIs:
10.1039/C9CP01716J
Source: RIS
Source ID: urn:123C3607C611BE5E25AFE8F4A1CACD57
Research output: Contribution to journal › Journal article – Annual report year: 2019 › Research › peer-review

Spin adapted implementation of EOM-CCSD for triplet excited states: Probing intersystem crossings of acetylacetone at the carbon and oxygen K-edges

We present an equation of motion coupled cluster singles and doubles approach for computing transient absorption spectra from a triplet excited state. The implementation determines the left and right excitation vectors by explicitly spin-adapting the triplet excitation space. As an illustrative application, we compute transient state X-ray absorption spectra at the carbon and oxygen K-edges for the acetylacetone molecule.

General information
Publication status: Published
Organisations: Department of Chemistry, Norwegian University of Science and Technology
Corresponding author: Coriani, S.
Contributors: Faber, R., Kjønstad, E. F., Koch, H., Coriani, S.
Number of pages: 10
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 151
The absorption spectrum of guanine based radicals: a comparative computational analysis

The excited states of the three radical derivatives of guanine, i.e. guanine cation (G⁺) and its two main deprotonated derivatives (G-H₁ and G-H₂) have been characterized in the Franck-Condon region by TD-DFT, using different functionals, CASPT2, and EOM-EE-CCSD calculations. In the gas phase, all the methods provide a similar description of the main spectral features, the pictures provided by TD-DFT, with long range corrected functionals, and EOM-EE-CCSD being very close. Solvent effects are then taken into account by a mixed discrete-continuum approach, including five water molecules of the first solvation shell and the Polarizable Continuum Model (PCM). The vibronic absorption line-width has finally been simulated at the TD-M052X level by a time dependent method within the harmonic approximation. The resulting absorption spectra are in good agreement with their experimental counterparts, providing useful indications on the use of PCM/TD-DFT based approaches to interpret the spectra of guanine based radicals within DNA.

The intriguing case of the one-photon and two-photon absorption of a prototypical symmetric squaraine: comparison of TDDFT and wave-function methods

We face the challenging description of the excited states responsible for one photon (OPA) and two photon (TPA) absorption in squaraine dyes, adopting both time-dependent density functional theory and a large variety of post Hartree Fock methods, including coupled cluster and adiabatic diagrammatic construction methods (ADC, to the second and third order), symmetry adapted cluster configuration interaction (CI), CASSCF including second-order perturbative corrections (PT2) with standard CASPT2 recipe and according to n-electron valence PT2 (NEVPT2) approach, and an additional multireference CI with PT2 corrections (CI-MRPT2). We selected a small prototypical symmetric squaraine dye for which these accurate computations are feasible and experimental data are available. We show that while all methods reasonably reproduce the OPA spectrum, an acceptable description and assignment of the states responsible for TPA is only possible through ADC(3) and multireference calculations, due to the strong involvement of double-excitations. The nature of ground state and OPA and TPA states is investigated with a rigorous reading of the CASSCF wavefunctions in terms of localized molecular orbitals on the donor and acceptor fragments, showing that these states arise from a balance of many different contributions including biradical configurations, local excitations and charge-transfer states where both side aromatic rings and the carbonyls of the squarylium moiety act as donors.
Time-resolved near-edge X-ray absorption fine structure of pyrazine from electronic structure and nuclear wave packet dynamics simulations

As a demonstration of the analysis of the electronic structure and the nuclear dynamics from time-resolved near-edge X-ray absorption fine structure (TR-NEXAFS), we present the TR-NEXAFS spectra of pyrazine following the excitation to the $1B_{2u}(\pi\pi^*)$ state. The spectra are calculated combining the frozen-core/core-valence separated equation-of-motion coupled cluster singles and doubles approach for the spectral signatures and the multiconfiguration time-dependent Hartree method for the wave packet propagation. The population decay from the $1B_{2u}(\pi\pi^*)$ state to the $1B_{3u}(\pi\pi^*)$ and $1A_u(n\pi^*)$ states, followed by oscillatory flow of population between the $1B_{3u}(\pi\pi^*)$ and $1A_u(n\pi^*)$ states, is interpreted by means of visualization of the potential energy curves and the reduced nuclear densities. By examining the electronic structure of the three valence-excited states and the final core-excited states, we observe that the population dynamics is explicitly reflected in the TR-NEXAFS spectra, especially when the heteroatoms are selected as the X-ray absorption sites. This work illustrates the feasibility of extracting fine details of molecular photophysical processes from TR-NEXAFS spectra by using currently available theoretical methods.
program package for computing vertical excitation energies and Faraday B terms in an implicit solvent approximated by the conductor-like screening model (COSMO) at the CC2 level, we have investigated the solvent effects on the relative positions of the ππ* and nπ* electronic transitions in these three molecules and compared them to the corresponding vacuum results. In the case of adenine we included also specific solvent effects with a small water cluster. The spectra obtained with the implicit model COSMO are in qualitative agreement with those obtained with explicit water molecules both with and without inclusion of the bulk solvent effects via the continuum solvent model. This suggests that the inclusion of the electrostatic contributions of the solvent can provide a sufficiently accurate description of the absorption spectra for adenine. The results for purine, adenine, and guanine show that after the inclusion of bulk solution the ππ* states shift to lower energies while at the same time nπ* states show a reversed behavior. The computed MCD spectra show the characteristic bi-signate profile found experimentally in all cases, despite, for adenine, remarkable differences in the origin of the individual peaks for different computational methods. Therefore, the ability (or inability) of MCD for determining the relative stability of the La and Lb states is critically re-assessed. According to our best estimate for adenine in aqueous solution the L_a state is more stable than L_b.

General information
Publication status: Published
Organisations: Department of Chemistry, Consiglio Nazionale delle Ricerche, Ruhr-Universität Bochum
Corresponding author: Coriani, S.
Contributors: Karbalaei Khani, S., Faber, R., Santoro, F., Hattig, C., Coriani, S.
Number of pages: 13
Pages: 1242-1254
Publication date: 2019
Peer-reviewed: Yes

Publication Information
Journal: Journal of Chemical Theory and Computation
Volume: 15
Issue number: 2
ISSN (Print): 1549-9618
Ratings:

A theoretical and experimental benchmark study of core-excited states in nitrogen
vibrational structure of the core-excited states. This makes nitrogen well suited for assessing the accuracy of different electronic structure methods for core excitations. We report high resolution experimental measurements performed at the SOLEIL synchrotron facility. These are compared with theoretical spectra calculated using coupled cluster theory and algebraic diagrammatic construction theory. The coupled cluster singles and doubles with perturbative triples model known as CC3 is shown to accurately reproduce the experimental excitation energies as well as the spacing of the vibrational transitions. The computational results are also shown to be systematically improved within the coupled cluster hierarchy, with the coupled cluster singles, doubles, triples, and quadruples method faithfully reproducing the experimental vibrational structure.

General information
Publication status: Published
Organisations: Department of Chemistry, University of Oslo, Stanford University, Johns Hopkins University, Synchrotron Soleil, Norwegian University of Science and Technology
Corresponding author: Koch, H.
Number of pages: 7
Publication date: 2018
Peer-reviewed: Yes

Publication Information
Journal: Journal of Chemical Physics
Volume: 148
Issue number: 6
Article number: 064106
ISSN (Print): 0021-9606
Developing theoretical beamlines for local, ultrafast and magnetic-field induced spectroscopic effects

General information
Publication status: Published
Organisations: Department of Chemistry
Contributors: Coriani, S., Lopez Vidal, M., Faber, R.
Publication date: 2018
Peer-reviewed: Yes
Event: Abstract from 16th International Congress of Quantum Chemistry, Menton, France.
Electronic versions: 16_icqc_abstract_lecture_coriani.pdf
Research output: Contribution to conference » Conference abstract for conference – Annual report year: 2018 » Research » peer-review

Investigations of natural and magnetically induced chirality via response theory methods

General information
Publication status: Published
Organisations: Department of Chemistry
Contributors: Coriani, S.
Publication date: 2018
Peer-reviewed: Yes
Publication information
Journal: Abstract of Papers of the American Chemical Society
Volume: 255
ISSN (Print): 0065-7727
Ratings:
Web of Science (2018): Indexed yes
Original language: English
Source: FindIt
Source ID: 2439061226
Research output: Contribution to journal » Conference abstract in journal – Annual report year: 2018 » Research » peer-review

Modeling magnetic circular dichroism within the polarizable embedding approach
Magnetic circular dichroism (MCD) is defined as the differential absorption of left and right circularly polarized light in a sample subjected to an external magnetic field. In order to interpret the results of MCD measurements, theoretical predictions of key MCD parameters can be of utmost importance. From an experimental point of view, MCD spectra of molecules are often measured in an environment and most notably in a solution. Thus, it may be very important that the method used to predict the MCD parameters is able to correctly account for medium effects. In this paper, we investigate the quality of MCD calculations within the polarizable embedding approach, which represents a fully atomistic and polarizable representation of an environment surrounding a smaller region treated using quantum mechanics. Furthermore, we compare the performance of the polarizable embedding scheme to the use of the more conventional dielectric continuum approach. Results are presented for cytosine and hypoxanthine solvated in water.

General information
Publication status: Published
One-Photon Absorption Properties from a Hybrid Polarizable Density Embedding/Complex Polarization Propagator Approach for Polarizable Solutions

We present a formulation of the polarizable density embedding (PDE) method in combination with the complex polarization propagator (CPP) method for the calculation of absorption spectra of molecules in solutions. The method is particularly useful for the calculation of near-edge X-ray absorption fine structure (NEXAFS) spectra. We compare the performance of PDE-CPP with the previously formulated polarizable embedding (PE)-CPP model for the calculation of the NEXAFS spectra of adenine, formamide, glycine, and adenosine triphosphate (ATP) in water at the carbon and nitrogen K-edges, as well as of formamide and glycine at the oxygen K-edge. In general, we find only minor differences between the performance of PDE and PE for the targeted parts of the spectra, except in the case of transitions involving Rydberg states, for which nonelectrostatic effects are found to be important.

General information
Publication status: Published
Organisations: Department of Chemistry, University of Southern Denmark
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Pages: 2145-2154
Publication date: 2018
Peer-reviewed: Yes
Developing Theoretical “Beamlines” for Modern Experiments

General information
Publication status: Published
Organisations: Department of Chemistry
Contributors: Coriani, S.
Publication date: 2017
Peer-reviewed: Yes
Event: Abstract from The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany.
Electronic versions:
WATOC_Abstract_Coriani.pdf

Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution
The excited electronic states of 2-thiouracil, 4-thiouracil and 2,4-dithiouracil, the analogues of uracil where the carbonyl oxygens are substituted by sulphur atoms, have been investigated by computing the magnetic circular dichroism (MCD) and one-photon absorption (OPA) spectra at the time-dependent density functional theory level. Special attention has been paid to solvent effects, included by a mixed discrete/continuum model, and to determining how our results depend on the adopted DFT functional (CAM-B3LYP and B3LYP). Whereas including solvent effects does not dramatically impact the MCD and OPA spectra, though improving the agreement with the experimental spectra, the performances of CAM-B3LYP and B3LYP are remarkably different. CAM-B3LYP captures well the effect of thionation on the uracil excited states and provides spectra in good agreement with the experiments, whereas B3LYP shows some deficiency in describing 2-TU and 2,4-DTU spectra, despite being more accurate than CAM-B3LYP for 4-TU.

Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution

General information
Publication status: Published
Organisations: Department of Chemistry, Consiglio Nazionale delle Ricerche, KTH - Royal Institute of Technology
Contributors: Martínez-Fernández, L., Fahleson, T., Norman, P., Santoro, F., Coriani, S., Improta, R.
Pages: 1415-1423
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Photochemical & Photobiological Sciences
Volume: 16
Issue number: 9
ISSN (Print): 1474-905X
Ratings:
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.77 SJR 0.818 SNIP 0.85
Web of Science (2017): Impact factor 2.902
Web of Science (2017): Indexed yes
Original language: English
Electronic versions:
Version4DTU.pdf. Embargo ended: 12/07/2018
DOIs:
10.1039/c7pp00105c
Source: FindIt
Source ID: 2372606155

Probing ultrafast ππ*/nπ* internal conversion in organic chromophores via K-edge resonant absorption
Many photoinduced processes including photosynthesis and human vision happen in organic molecules and involve coupled femtosecond dynamics of nuclei and electrons. Organic molecules with heteroatoms often possess an important excited-state relaxation channel from an optically allowed ππ* to a dark nπ* state. The ππ*/nπ* internal conversion is difficult to investigate, as most spectroscopic methods are not exclusively sensitive to changes in the excited-state electronic structure. Here, we report achieving the required sensitivity by exploiting the element and site specificity of near-
edge soft X-ray absorption spectroscopy. As a hole forms in the \( n \) orbital during \( \pi^+\pi^- \) internal conversion, the absorption spectrum at the heteroatom K-edge exhibits an additional resonance. We demonstrate the concept using the nucleobase thymine at the oxygen K-edge, and unambiguously show that \( \pi^+\pi^- \) internal conversion takes place within (60 +/- 30) fs. High-level-coupled cluster calculations confirm the method's impressive electronic structure sensitivity for excited-state investigations.

**General information**
Publication status: Published
Organisations: Department of Chemistry, SLAC National Accelerator Laboratory, University of Gothenburg, University of Connecticut, Swiss Federal Institute of Technology Lausanne, Uppsala University, Sincrotrone Trieste
Publication date: 2017
Peer-reviewed: Yes

**Publication information**
Journal: Nature Communications
Volume: 8
Issue number: 1
Article number: 29
ISSN (Print): 2041-1723
Ratings:
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.934
Web of Science (2017): Impact factor 12.353
Web of Science (2017): Indexed yes
Original language: English
Keywords: Atomic and molecular interactions with photons, Chemical physics
Electronic versions:
redirect_nature.pdf
DOIs:
10.1038/s41467-017-00069-7

**Bibliographical note**
This article is licensed under a Creative Commons Attribution 4.0 International License.
Source: FindIt
Source ID: 2371607311
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review

**Relation between molecular electronic structure and nuclear spin-induced circular dichroism**
The recently theoretically described nuclear spin-induced circular dichroism (NSCD) is a promising method for the optical detection of nuclear magnetization. NSCD involves both optical excitations of the molecule and hyperfine interactions and, thus, it offers a means to realize a spectroscopy with spatially localized, high-resolution information. To survey the factors relating the molecular and electronic structure to the NSCD signal, we theoretically investigate NSCD of twenty structures of the four most common nucleic acid bases (adenine, guanine, thymine, cytosine). The NSCD signal correlates with the spatial distribution of the excited states and couplings between them, reflecting changes in molecular structure and conformation. This constitutes a marked difference to the nuclear magnetic resonance (NMR) chemical shift, which only reflects the local molecular structure in the ground electronic state. The calculated NSCD spectra are rationalized by means of changes in the electronic density and by a sum-over-states approach, which allows to identify the contributions of the individual excited states. Two separate contributions to NSCD are identified and their physical origins and relative magnitudes are discussed. The results underline NSCD spectroscopy as a plausible tool with a power for the identification of not only different molecules, but their specific structures as well.

**General information**
Publication status: Published
Organisations: Department of Chemistry, University of Oulu, University of Helsinki
Contributors: Štěpánek, P., Coriani, S., Sundholm, D., Ovchinnikov, V. A., Vaara, J.
Number of pages: 11
Publication date: 2017
Peer-reviewed: Yes

**Publication information**
Journal: Scientific Reports
Zeeman effect in sulfur monoxide: a tool to probe magnetic fields in star forming regions

Context. Magnetic fields play a fundamental role in star formation processes and the best method to evaluate their intensity is to measure the Zeeman effect of atomic and molecular lines. However, a direct measurement of the Zeeman spectral pattern from interstellar molecular species is challenging due to the high sensitivity and high spectral resolution required. So far, the Zeeman effect has been detected unambiguously in star forming regions for very few non-masing species, such as OH and CN. Aims. We decided to investigate the suitability of sulfur monoxide (SO), which is one of the most abundant species in star forming regions, for probing the intensity of magnetic fields via the Zeeman effect. Methods. We investigated the Zeeman effect for several rotational transitions of SO in the (sub-)mm spectral regions by using a frequency-modulated, computer-controlled spectrometer, and by applying a magnetic field parallel to the radiation propagation (i.e., perpendicular to the oscillating magnetic field of the radiation). To support the experimental determination of the g factors of SO, a systematic quantum-chemical investigation of these parameters for both SO and O₂ has been carried out. Results. An effective experimental-computational strategy for providing accurate g factors as well as for identifying the rotational transitions showing the strongest Zeeman effect has been presented. Revised g factors have been obtained from a large number of SO rotational transitions between 86 and 389 GHz. In particular, the rotational transitions showing the largest Zeeman shifts are: N,J = 2, 2 ← 1, 1 (86.1 GHz), N,J = 4, 3 ← 3, 2 (159.0 GHz), N,J = 1, 1 ← 0, 1 (286.3 GHz), N,J = 2, 2 ← 1, 2 (309.5 GHz), and N,J = 2, 1 ← 1, 0 (329.4 GHz). Our investigation supports SO as a good candidate for probing magnetic fields in high-density star forming regions.
A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion

A computational protocol for magneto-chiral dichroism and magneto-chiral birefringence dispersion is presented within the framework of damped response theory, also known as complex polarization propagator theory, at the level of time-dependent Hartree-Fock and time-dependent density functional theory. Magneto-chiral dichroism and magneto-chiral birefringence spectra in the (resonant) frequency region below the first ionization threshold of R-methyloxirane and L-alanine are presented and compared with the corresponding results obtained for both the electronic circular dichroism and the magnetic circular dichroism. The additional information content yielded by the magneto-chiral phenomena, as well as their potential experimental detectability for the selected species, is discussed.

A study of the valence shell electronic states of s-triazine by photoabsorption spectroscopy and ab initio calculations

The absolute photoabsorption cross section of s-triazine has been measured between 4 and 40 eV, and is dominated by bands associated with valence states. Structure due to Rydberg excitations is both weak and irregular. Jahn-Teller interactions affect the vibronic structure observed in the Rydberg absorption bands due to excitation from the 1e'' or 6e'' orbitals. The interpretation of the experimental spectrum has been guided by transition energies and oscillator strengths, for Rydberg and valence states, calculated with the time-dependent version of density functional theory and with the coupled cluster linear response approach. The theoretical studies indicate that Rydberg/Rydberg and Rydberg/valence mixing is important. (C) 2016 Elsevier B.V. All rights reserved.
Coupled Cluster Study of Photoionization and Photodetachment Cross Sections

To simulate photoionization and photodetachment cross sections, as well as polarizability dispersion profiles below the ionization threshold, a discretized (pseudo)-spectrum stretching over the entire frequency region (including the continuum) obtained from an asymmetric Lanczos algorithm at the coupled cluster singles and doubles level is used to reconstruct the complex dipole polarizability, on which an analytic continuation procedure is then applied. Through a suitable selection of points in the complex plane, which we have shown can be quite general, we were able to perform an analytical continuation procedure. Results are reported for atoms He and Ne, molecules H-2, N-2, CH4, H2CO, C2H2, CO2, CO, H2O, NH3, and SO2, and anions H-, F-, OH-, and NH2-. The method employed has proved to work well with a rather small Lanczos chain length as well as with medium-sized correlation consistent basis sets supplemented with a limited number of continuum-like Gaussian functions. Such features suggest the applicability of the method to larger systems.

Erratum: *Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework*
Molecular Dipole Moments within the Incremental Scheme Using the Domain-Specific Basis-Set Approach
We present the first implementation of the fully automated incremental scheme for CCSD unrelaxed dipole moments using the domain-specific basis-set approach. Truncation parameters are varied, and the accuracy of the method is statistically analyzed for a test set of 20 molecules. The local approximations introduce small errors at second order and negligible ones at third order. For a third-order incremental CCSD expansion with a CC2 error correction, a cc-pVDZ/SV domain-specific basis set (t_{\text{main}} = 3.5 Bohr), and the truncation parameter f = 30 Bohr, we obtain a mean error of 0.00 mau (-0.20 mau) and a standard deviation of 1.95 mau (2.17 mau) for the total dipole moments (Cartesian components of the dipole vectors). By analyzing incremental CCSD energies, we demonstrate that the MP2 and CC2 error correction schemes are an exclusive correction for the domain-specific basis-set error. Our implementation of the incremental scheme provides fully automated computations of highly accurate dipole moments at reduced computational cost and is fully parallelized in terms of the calculation of the increments. Therefore, one can utilize the incremental scheme, on the same hardware, to extend the basis set in comparison to standard CCSD and thus obtain a better total accuracy.

Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective
Molecular response properties for ground and excited states and for transitions between these states are defined by solving the time-dependent Schrodinger equation for a molecular system in a field of a time-periodic perturbation. In equation of motion coupled cluster (EOM-CC) theory, molecular response properties are commonly obtained by replacing, in configuration interaction (CI) molecular response property expressions, the energies and eigenstates of the CI eigenvalue equation with the energies and eigenstates of the EOM-CC eigenvalue equation. We show here that EOM-CC molecular response properties are identical to the molecular response properties that are obtained in the coupled cluster-configuration interaction (CC-CI) model, where the time-dependent Schrodinger equation is solved using an exponential (coupled cluster) parametrization to describe the unperturbed system and a linear (configuration interaction) parametrization to describe the time evolution of the unperturbed system. The equivalence between EOM-CC and CC-CI molecular response properties only holds when the CI molecular response property expressions-from which the EOM-CC
expressions are derived—are determined using projection and not using the variational principle. In a previous article [F. Pawlowski, J. Olsen, and P. Jørgensen, J. Chem. Phys. 142, 114109 (2015)], it was stated that the equivalence between EOM-CC and CC-CI molecular response properties only held for a linear response function, whereas quadratic and higher order response functions were mistakenly said to differ in the two approaches. Proving the general equivalence between EOM-CC and CC-CI molecular response properties is a challenging task, that is undertaken in this article. Proving this equivalence not only corrects the previous incorrect statement but also first and foremost leads to a new, time-dependent, perspective for understanding the basic assumptions on which the EOM-CC molecular response property expressions are founded. Further, the equivalence between EOM-CC and CC-CI molecular response properties highlights how static molecular response properties can be obtained from finite-field EOM-CC energy calculations.

Near-Edge X-ray Absorption Fine Structure within Multilevel Coupled Cluster Theory

Core excited states are challenging to calculate, mainly because they are embedded in a manifold of high energy valence-excited states. However, their locality makes their determination ideal for local correlation methods. In this paper, we demonstrate the performance of multilevel coupled cluster theory in computing core spectra both within the core valence separated and the asymmetric Lanczos implementations of coupled cluster linear response theory. We also propose a visualization-tool to analyze the excitations using the difference between the ground-state and excited-state electron densities.

General information
Publication status: Published
Organisations: Norwegian University of Science and Technology, University of Trieste, Aarhus University, Stanford University
Requirements of first-principles calculations of X-ray absorption spectra of liquid water

A computational benchmark study on X-ray absorption spectra of water has been performed by means of transition-potential density functional theory (TP-DFT), damped time-dependent density functional theory (TDDFT), and damped coupled cluster (CC) linear response theory. For liquid water, using TDDFT with a tailored CAM-B3LYP functional and a polarizable embedding, we find that an embedding with over 2000 water molecules is required to fully converge spectral features for individual molecules, but a substantially smaller embedding can be used within averaging schemes. TP-DFT and TDDFT calculations on 100 MD structures demonstrate that TDDFT produces a spectrum with spectral features in good agreement with experiment, while it is more difficult to fully resolve the spectral features in the TP-DFT spectrum. Similar trends were also observed for calculations of bulk ice. In order to further establish the performance of these methods, small water clusters have been considered also at the CC2 and CCSD levels of theory. Issues regarding the basis set requirements for spectrum simulations of liquid water and the determination of gas-phase ionization potentials are also discussed.
A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption

We present a computational methodology to calculate the intensity of circular dichroism (CD) in spin-forbidden absorption and of circularly polarized phosphorescence (CPP) signals, a manifestation of the optical activity of the triplet–singlet transitions in chiral compounds. The protocol is based on the response function formalism and is implemented at the level of time-dependent density functional theory. It has been employed to calculate the spin-forbidden circular dichroism and circularly polarized phosphorescence signals of valence $n \rightarrow p^*$ and $n \leftarrow p^*$ transitions, respectively, in several chiral enones and diketones. Basis set effects in the length and velocity gauge formulations have been explored, and the accuracy achieved when employing approximate (mean-field and effective nuclear charge) spin–orbit operators has been investigated. CPP is shown to be a sensitive probe of the triplet excited state structure. In many cases the sign of the spin-forbidden CD and CPP signals are opposite. For the b,g-enones under investigation, where there are two minima on the lowest triplet excited state potential energy surface, each minimum exhibits a CPP signal of a different sign.

General information
Publication status: Published
Organisations: University of Warsaw, Consiglio Nazionale delle Ricerche, University of Trieste, Aarhus University
Contributors: Kaminski, M., Cukras, J., Pecul, M., Rizzoc, A., Coriani, S.
Number of pages: 8
Pages: 19079-19086
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 17
Issue number: 29
ISSN (Print): 1463-9076
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.188
Web of Science (2015): Indexed yes
Original language: English
DOIs:
10.1039/c5cp02590g
Source: FindIt
Source ID: 2266152870
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

A study of the valence shell electronic structure and photoionisation dynamics of s-triazine

A joint experimental and theoretical approach has been used to study the valence shell electronic structure and photoionisation dynamics of s-triazine (1,3,5-triazine). Synchrotron radiation has been employed to record angle resolved photoelectron spectra of the complete valence shell for photon energies between 17.5 and 100 eV, thereby allowing photoelectron anisotropy parameters and branching ratios to be determined. Absolute photoionisation partial cross sections have been estimated as the product of these branching ratios and the absolute photoabsorption cross section. The Kohn-Sham and the time-dependent version of density functional theory methods have been used to calculate photoelectron anisotropy parameters and photoionisation partial cross sections, and these have been compared with the corresponding experimental data. The calculations predict that shape resonances affect the photoionisation dynamics of several of the molecular orbitals. The angle resolved photoelectron spectra suggest that the $1a_{2u}'(n)$ orbital is more tightly bound than the $5e'(\sigma)$ orbital, and that the $4a_1'(\sigma)$ orbital is more tightly bound than the $1a_2'(\sigma)$ orbital, in agreement with the predicted molecular orbital sequence. For the outer valence orbitals the single-particle picture of ionisation holds but electron correlation becomes increasingly important for the inner valence $4e'$, $3e'$ and $3a_1'$ orbitals and leads to a redistribution of intensity. Instead of a readily distinguishable main-line, associated with each of these orbitals, the photoelectron intensity is spread over numerous satellite states and the resulting band is broad and featureless.

General information
Publication status: Published
Organisations: University of Trieste, Daresbury Laboratory, King's College London, Uppsala University
Contributors: Coriani, S., Stener, M., Decleva, P., Holland, D. M. P., Potts, A. W., Karlsson, L.
Number of pages: 10
Pages: 115-124
Publication date: 2015
Peer-reviewed: Yes

Publication information
Circular and linear magnetic birefringences in xenon at $\lambda=1064$ nm

The circular and linear magnetic birefringences corresponding to the Faraday and the Cotton-Mouton effects, respectively, have been measured in xenon at $\lambda=1064$ nm. The experimental setup is based on time dependent magnetic fields and a high finesse Fabry-Perot cavity. Our value of the Faraday effect is the first measurement at this wavelength. It is compared to theoretical predictions. Our uncertainty of a few percent yields an agreement at better than 1σ with the computational estimate when relativistic effects are taken into account. Concerning the Cotton-Mouton effect, our measurement, the second ever published at $\lambda=1064$ nm, agrees at better than 1σ with theoretical predictions. We also compare our error budget with that established for other experimental published values.

General information

Publication status: Published
Organisations: Laboratoire National de Champs Magnétiques Intenses, Consiglio Nazionale delle Ricerche, University of Trieste, Aarhus University
Contributors: Cadene, A., Fouche, M., Rivere, A., Battesti, R., Coriani, S., Rizzo, A., Rizzo, C.
Number of pages: 10
Publication date: 2015
Peer-reviewed: Yes

Publication information

Journal: Journal of Chemical Physics
Volume: 142
Issue number: 12
Article number: 124313
ISSN (Print): 0021-9606
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 1.042
Web of Science (2015): Impact factor 2.894
Web of Science (2015): Indexed yes
Original language: English
Electronic versions:
2015_JCP_Cadene_Xenon.pdf
DOIs:
10.1063/1.4916049

Bibliographical note
© 2015 AIP Publishing LLC.
Source: FindIt
Source ID: 2264432457
Research output: Contribution to journal » Journal article – Annual report year: 2015 » Research » peer-review

Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework
We present a simple scheme to compute X-ray absorption spectra (e.g., near-edge absorption fine structure) and core ionisation energies within coupled cluster linear response theory. The approach exploits the so-called core-valence separation to effectively reduce the excitation space to processes involving at least one core orbital, and it can be easily implemented within any pre-existing coupled cluster code for low energy states. We further develop a perturbation correction that incorporates the effect of the excluded part of the excitation space. The correction is shown to be highly accurate. Test results are presented for a set of molecular systems for which well converged results in full space could be generated at the coupled cluster singles and doubles level of theory only, but the scheme is straightforwardly generalizable to all members of the coupled cluster hierarchy of approximations, including CC3.

**General information**
Publication status: Published
Organisations: Norwegian University of Science and Technology, University of Trieste, Aarhus University
Contributors: Coriani, S., Koch, H.
Number of pages: 6
Publication date: 2015
Peer-reviewed: Yes

**Publication Information**
Journal: Journal of Chemical Physics
Volume: 143
Issue number: 18
Article number: 181103
ISSN (Print): 0021-9606
Ratings:
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 1.98 SJR 1.255 SNIP 1.042
- Web of Science (2015): Impact factor 2.894
- Web of Science (2015): Indexed yes
Original language: English
Electronic versions:
- 2015_JCP_Coriani_CVSCC.pdf
- 10.1063/1.4935712

**Bibliographical note**
© 2015 AIP Publishing LLC.
Source: FindIt
Source ID: 2287989937
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

**TD-DFT Investigation of the Magnetic Circular Dichroism Spectra of Some Purine and Pyrimidine Bases of Nucleic Acids**
We present a computational study of the Magnetic circular dichroism (MCD) spectra in the 200-300 nm wavelength region of purine and its derivative hypoxanthine, as well as of the pyrimidine bases of nucleic acids uracil, thymine, and cytosine, Using the B3LYP and CAM-B3LYP functionals. Solvent effects, are investigated within the polarizable continuum model and by inclusion of explicit water molecules. In, general; the computed spectra are found to be in good agreement with the experimental ones, apart from some overall blue shifts. Both the pseudo-A term shape of the MCD spectra of the purines and the B term shape of the spectra of pyrimidine base are reproduced. Our calculations also correctly reproduce the reversed phase of the MCD bands in purine compared to, that of its derivatives present in nucleic acids. Solvent effects are sizable and system specific, but they do not in general alter the qualitative shape of the spectra. The bands are dominated the-bright pi -> pi* transitions; and our calculations in solution nicely reproduce the energy differences, improving the estimates obtained in the gas phase. Shoulders are predicted for purine and uracil due to n -> pi* excitations, but they are too weak to be observed in the experiment.

**General information**
Publication status: Published
Organisations: Linköping University, Istituto di Chimica dei Composti Organometallic, Istituto di Biostrutture e Bioimmagini, University of Trieste, Aarhus University
Contributors: Fahleson, T., Kauczor, J., Norman, P., Santoro, F., Improta, R., Coriani, S.
Number of pages: 14
Pages: 5476-5489
Publication date: 2015
Peer-reviewed: Yes

**Publication Information**
A coupled-cluster study of photodetachment cross sections of closed-shell anions

We investigate the performance of Stieltjes Imaging applied to Lanczos pseudo-spectra generated at the coupled cluster singles and doubles, coupled cluster singles and approximate iterative doubles and coupled cluster singles levels of theory in modeling the photodetachment cross sections of the closed shell anions H−, Li−, Na−, F−, Cl−, and OH−. The accurate description of double excitations is found to play a much more important role than in the case of photoionization of neutral species. (C) 2014 AIP Publishing LLC.

General information
Publication status: Published
Organisations: University of Trieste
Contributors: Cukras, J., Decleva, P., Coriani, S.
Number of pages: 12
Publication date: 2014
Peer-reviewed: Yes

Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H₂ molecule
Using an asymmetric Lanczos chain algorithm for the calculation of the coupled cluster linear response functions at the coupled cluster singles and doubles (CCSD) and coupled cluster singles and approximate iterative doubles (CC2) levels of approximation, we have calculated the mean excitation energies of the noble gases He, Ne and Ar, and of the hydrogen molecule (H₂). Convergence with respect to the one-electron basis set was investigated in detail for families of correlation-consistent basis sets including both augmentation and core-valence functions. We find that the electron correlation effects at the CCSD level change the mean excitation energies obtained at the uncorrelated Hartree-Fock level by about 1%. For the two-electron systems He and H₂, our CCSD results (for a Lanczos chain length equal to the full excitation space), I₀ = 42.28 eV (helium) and I₀ = 19.62 eV (H₂), correspond to full configuration interaction results and are therefore the exact, non-relativistic theoretical values for the mean excitation energy of these two systems within the Bethe theory for the chosen basis set and, in the case of H₂, at the experimental equilibrium geometry.

General information
Dynamical photoionization observables of the CS molecule: The role of electron correlation
Highly correlated calculations are performed on the primary ionic states and the prominent satellite present in the outer valence photoelectron spectrum of carbon monosulfide (CS). Dyson orbitals are coupled to accurate one particle continuum orbitals to provide a correlated description of energy dependent cross sections, asymmetry parameters, branching ratios, and molecular frame photoelectron angular distributions. The comparison with results obtained at the Hartree-Fock and Density Functional Theory level shows the strong sensitivity of these observables to details of the correlation in the bound states. The behaviour of the well characterized satellite state is analyzed in detail, and shows differences from the relevant primary states, revealing the limitations of a simple intensity borrowing mechanism. The results resolve the intensity disagreement with experiment obtained at the level of the sudden approximation. © 2014 AIP Publishing LLC.

General information
Publication status: Published
Organisations: University of Trieste, University of Ferrara
Contributors: Ponzi, A., Angeli, C., Cimiraglia, R., Coriani, S., Decleva, P.
Number of pages: 11
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 140
Issue number: 20
Article number: 204304
ISSN (Print): 0021-9606
Ratings:
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.029
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
Original language: English
DOIs:
10.1063/1.4876495
Source: FindIt
Source ID: 267986916
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review
**Identifying the Hamiltonian structure in linear response theory**

We present a unifying framework for linear response eigenvalue equations that encompasses both variational Hartree-Fock and Kohn-Sham density functional theory as well as non-variational coupled-cluster theory. The joint description is rooted in the so-called Hamiltonian structure of the response kernel matrices, whose properties permit an immediate identification of the well-known paired eigenvalue spectrum describing a molecule in the isolated state. Recognizing the Hamiltonian structure underlying the equations further enables a generalization to the case of a polarizable-embedded molecule treated in variational and, in particular, in non-variational theories. © 2014 AIP Publishing LLC.

**General information**

Publication status: Published
Organisations: University of Southern Denmark, Aarhus University, University of Trieste
Contributors: List, N. H., Coriani, S., Christiansen, O., Kongsted, J.
Number of pages: 6
Publication date: 2014
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Chemical Physics
Volume: 140
Issue number: 22
Article number: 224103
ISSN (Print): 0021-9606
Ratings:
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.029
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
Original language: English
DOI:
10.1063/1.4881145
Source: FindIt
Source ID: 268205510
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review

**Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments**

We present an extension of a previously reported implementation of a Lanczos-driven coupled-cluster (CC) damped linear response approach to molecules in condensed phases, where the effects of a surrounding environment are incorporated by means of the polarizable embedding formalism. We are specifically motivated by a twofold aim: (i) computation of core excitations in realistic surroundings and (ii) examination of the effect of the differential response of the environment upon excitation solely related to the CC multipliers (herein denoted the J matrix) in computations of excitation energies and transition moments of polarizable-embedded molecules. Numerical calculations demonstrate that the differential polarization of the environment due to the first-order CC multipliers provides only minor contributions to the solvatochromic shift for all transitions considered. We thus complement previous works by confirming numerically the validity of the routinely invoked neglect of the J matrix contribution as well as motivating future use of the approximation that offers a reduction of the dimensionality of the eigenvalue problem. Preliminary applications to K-edge absorption of liquid water and aqueous acrolein are presented and highlight the importance of the environment that gives rise to transition-specific shifts. (c) 2014 AIP Publishing LLC.

**General information**

Publication status: Published
Organisations: University of Southern Denmark, Aarhus University, University of Trieste
Contributors: List, N. H., Coriani, S., Kongsted, J., Christiansen, O.
Number of pages: 13
Publication date: 2014
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Chemical Physics
Volume: 141
Issue number: 24
Article number: 244107
ISSN (Print): 0021-9606
Ratings:
Nuclear spin circular dichroism

Recent years have witnessed a growing interest in magneto-optic spectroscopy techniques that use nuclear magnetization as the source of the magnetic field. Here we present a formulation of magnetic circular dichroism (CD) due to magnetically polarized nuclei, nuclear spin-induced CD (NSCD), in molecules. The NSCD ellipticity and nuclear spin-induced optical rotation (NSOR) angle correspond to the real and imaginary parts, respectively, of (complex) quadratic response functions involving the dynamic second-order interaction of the electron system with the linearly polarized light beam, as well as the static magnetic hyperfine interaction. Using the complex polarization propagator framework, NSCD and NSOR signals are obtained at frequencies in the vicinity of optical excitations. Hartree-Fock and density-functional theory calculations on relatively small model systems, ethene, benzene, and 1,4-benzoquinone, demonstrate the feasibility of the method for obtaining relatively strong nuclear spin-induced ellipticity and optical rotation signals. Comparison of the proton and carbon-13 signals of ethanol reveals that these resonant phenomena facilitate chemical resolution between non-equivalent nuclei in magneto-optic spectra. (C) 2014 AIP Publishing LLC.

General information
Publication status: Published
Organisations: University of Oulu, Consiglio Nazionale delle Ricerche, Linköping University, University of Trieste
Contributors: Vaara, J., Rizzo, A., Kauczor, J., Norman, P., Coriani, S.
Number of pages: 14
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 140
Issue number: 13
Article number: 134103
ISSN (Print): 0021-9606
Ratings:
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.54 SJR 1.446 SNIP 1.029
Web of Science (2014): Impact factor 2.952
Web of Science (2014): Indexed yes
Original language: English
DOIs:
10.1063/1.4869849
Source: FindIt
Source ID: 266724716
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review

Nuclear spin circular dichroism in fullerenes: a computational study

In the recently proposed phenomenon, nuclear spin-induced circular dichroism (NSCD), collective magnetisation of nuclei induces circular dichroism in a light beam passing through a molecular sample. Here we present the first computational predictions of NSCD for fullerenes C_{60} and C_{70}. We show that the NSCD signal is nucleus-specific, like in NMR spectroscopy. Thus, NSCD may provide a new and promising, high-resolution observable for experimental identification of chemical compounds.

General information
Publication status: Published
Organisations: Czech Academy of Sciences, University of Oulu, University of Trieste
Contributors: Straka, M., Stepanek, P., Coriani, S., Vaara, J.
Number of pages: 4
Relative Stability of the $L_a$ and $L_b$ Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra

The relative position of $L_a$ and $L_b$ ππ* electronic states in purine nucleobases is a much debated topic, since it can strongly affect our understanding of their photoexcited dynamics. To assess this point, we calculated the absorption and magnetic circular dichroism (MCD) spectra of adenine, guanine, and their nucleosides in gas-phase and aqueous solution, exploiting recent developments in MCD computational technology within time-dependent density functional theory. MCD spectroscopy allows us to resolve the intense $S_0 \rightarrow L_a$ transition from the weak $S_0 \rightarrow L_b$ transition. The spectra obtained in water solution, by using B3LYP and CAM-B3LYP functionals and describing solvent effect by cluster models and by the polarizable continuum model (PCM), are in very good agreement with the experimental counterparts, thus providing direct and unambiguous evidence that the energy ordering predicted by TD-DFT, $L_a < L_b$, is the correct one.

The Dalton quantum chemistry program system

Dalton is a powerful general-purpose program system for the study of molecular electronic structure at the Hartree-Fock, Kohn-Sham, multiconfigurational self-consistent-field, M0ller-Plesset, configuration-interaction, and coupled-cluster levels of theory. Apart from the total energy, a wide variety of molecular properties may be calculated using these electronic-
structure models. Molecular gradients and Hessians are available for geometry optimizations, molecular dynamics, and vibrational studies, whereas magnetic resonance and optical activity can be studied in a gauge-origin-invariant manner. Frequency-dependent molecular properties can be calculated using linear, quadratic, and cubic response theory. A large number of singlet and triplet perturbation operators are available for the study of one-, two-, and three-photon processes. Environmental effects may be included using various dielectric-medium and quantum-mechanics/molecular-mechanics models. Large molecules may be studied using linear-scaling and massively parallel algorithms. Dalton is distributed at no cost from a number of UNIX platforms.

General information
Publication status: Published
Organisations: University of Trieste, Aarhus University, University of Copenhagen, University of Southern Denmark, University of Oslo, Vilnius University, University of Ferrara, KTH - Royal Institute of Technology, Norwegian Computing Center, Systematic A/S, University of Santiago de Compostela, UiT The Arctic University of Norway
Number of pages: 16
Pages: 269-284
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Wiley Interdisciplinary Reviews: Computational Molecular Science
Volume: 4
Issue number: 3
ISSN (Print): 1759-0884
Scopus rating (2014): CiteScore 11.17 SJR 4.907 SNIP 3.973
Web of Science (2014): Impact factor 11.885
Original language: English
Electronic versions:
Aidas_et_al_2014_Wiley_Interdisciplinary_Reviews_Computational_Molecular_Science.pdf
DOI: 10.1002/wcms.1172

Bibliographical note
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Source: FindIt
Source ID: 255042836
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review

A density functional theory study of magneto-electric Jones birefringence of noble gases, furan homologues, and monosubstituted benzenes
We report on the results of a systematic ab initio study of the Jones birefringence of noble gases, of furan homologues, and of monosubstituted benzenes, in the gas phase, with the aim of analyzing the behavior and the trends within a list of systems of varying size and complexity, and of identifying candidates for a combined experimental/theoretical study of the effect. We resort here to analytic linear and nonlinear response functions in the framework of time-dependent density functional theory. A correlation is made between the observable (the Jones constant) and the atomic radius for noble gases, or the permanent electric dipole and a structure/chemical reactivity descriptor as the para Hammett constant for substituted benzenes.

General information
Publication status: Published
Organisations: Linköping University, University of Trieste, CNR, Universite Grenoble Alpes
Corresponding author: Rizzo, A.
Contributors: Fahleson, T., Norman, P., Coriani, S., Rizzo, A., Rikken, G. L. J. A.
Carbon X-ray absorption spectra of fluoroethenes and acetone: A study at the coupled cluster, density functional, and static-exchange levels of theory

Near carbon K-edge X-ray absorption fine structure spectra of a series of fluorine-substituted ethenes and acetone have been studied using coupled cluster and density functional theory (DFT) polarization propagator methods, as well as the static-exchange (STEX) approach. With the complex polarization propagator (CPP) implemented in coupled cluster theory, relaxation effects following the excitation of core electrons are accounted for in terms of electron correlation, enabling a systematic convergence of these effects with respect to electron excitations in the cluster operator. Coupled cluster results have been used as benchmarks for the assessment of propagator methods in DFT as well as the state-specific static-exchange approach. Calculations on ethene and 1,1-difluoroethene illustrate the possibility of using nonrelativistic coupled cluster singles and doubles (CCSD) with additional effects of electron correlation and relativity added as scalar shifts in energetics. It has been demonstrated that CPP spectra obtained with coupled cluster singles and approximate doubles (CC2), CCSD, and DFT (with a Coulomb attenuated exchange-correlation functional) yield excellent predictions of chemical shifts for vinylfluoride, 1,1-difluoroethene, trifluoroethene, as well as good spectral features for acetone in the case of CCSD and DFT. Following this, CPP-DFT is considered to be a viable option for the calculation of X-ray absorption spectra of larger π-conjugated systems, and CC2 is deemed applicable for chemical shifts but not for studies of fine structure features. The CCSD method as well as the more approximate CC2 method are shown to yield spectral features relating to π*-resonances in good agreement with experiment, not only for the aforementioned molecules but also for ethene, cis-1,2-difluoroethene, and tetrafluoroethene. The STEX approach is shown to underestimate π*-peak separations due to spectral compressions, a characteristic which is inherent to this method.
Communication: Analytic gradients in the random-phase approximation
The relationship between the random-phase-approximation (RPA) correlation energy and the continuous algebraic Riccati equation is examined and the importance of a stabilizing solution is emphasized. The criterion to distinguish this from non-stabilizing solutions can be used to ensure that physical, smooth potential energy surfaces are obtained. An implementation of analytic RPA molecular gradients is presented using the Lagrangian technique. Illustrative calculations indicate that RPA with Hartree-Fock reference orbitals delivers an accuracy similar to that of second-order Møller-Plesset perturbation theory.

General information
Publication status: Published
Organisations: University of Oslo, University of Trieste, University of Nottingham
Contributors: Rekkedal, J., Coriani, S., Iozzi, M. F., Teale, A. M., Helgaker, T., Pedersen, T. B.
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 139
Issue number: 8
Article number: 081101
ISSN (Print): 0021-9606
Ratings:
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.182

Communication: A reduced-space algorithm for the solution of the complex linear response equations used in coupled cluster damped response theory
We present a reduced-space algorithm for solving the complex (damped) linear response equations required to compute the complex linear response function for the hierarchy of methods: coupled cluster singles, coupled cluster singles and iterative approximate doubles, and coupled cluster singles and doubles. The solver is the keystone element for the development of damped coupled cluster response methods for linear and nonlinear effects in resonant frequency regions.

General information
Publication status: Published
Organisations: Linköping University, Aarhus University, University of Trieste
Contributors: Kauczor, J., Norman, P., Christiansen, O., Coriani, S.
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 139
Issue number: 21
Article number: 211102
ISSN (Print): 0021-9606
Ratings:
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.559 SNIP 1.182
On the Absolute Configuration of Chiral 1,4-Dihydropyridazines Synthesized by Organocatalysed Reactions

A computational investigation of the specific optical rotation and of the electronic circular dichroism spectra of two chiral 1,4-dihydropyridazines was performed and compared with existing experimental data to verify a previous assignment of their absolute configuration based on a well-accepted mechanism of catalysis of the organocatalyst used in their synthesis. Both the optical rotation and circular dichroism calculations indicate that the absolute configuration is opposite to the one assigned on the basis of the mechanism originally assumed. An alternative reaction mechanism is therefore suggested.

Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra

A recently implemented asymmetric Lanczos algorithm for computing (complex) linear response functions within the coupled cluster singles (CCS), coupled cluster singles and iterative approximate doubles (CC2), and coupled cluster singles and doubles (CCSD) is coupled to a Stieltjes imaging technique in order to describe the photoionization cross section of atoms and molecules, in the spirit of a similar procedure recently proposed by Averbukh and co-workers within the Algebraic Diagrammatic Construction approach. Pilot results are reported for the atoms He, Ne, and Ar and for the molecules H₂, H₂O, NH₃, HF, CO, and CO₂.
Ab initio calculation of magnetic circular dichroism
We discuss the ab initio calculation of all terms contributing to a magnetic circular dichroism (MCD) spectrum—i.e., A, B, and C terms—and give an overview of the most recent methods that have been introduced for calculating these different contributions. Among them, we highlight the use of the complex polarization propagator approach because it may give direct access to the A and B terms of MCD. We also briefly discuss how ab initio calculations for analyzing experimental MCD spectra can be used to gain insight into the electronic excited states of molecules.

Asymmetric-Lanczos-Chain-Driven Implementation of Electronic Resonance Convergent Coupled-Cluster Linear Response Theory
We present an implementation of the damped coupled-cluster linear response function based on an asymmetric Lanczos chain algorithm for the hierarchy of coupled-cluster approximations CCS (coupled-cluster singles), CC2 (coupled cluster singles and approximate doubles), and CCSD (coupled-cluster singles and doubles). Triple corrections to the excitation energies can be included via the CCSDR(3) (coupled-cluster singles and doubles with noniterative-triples-corrected excitation energies) approximation. The performance and some of the potentialities of the approach are investigated in calculations of the visible/ultraviolet absorption spectrum and the dispersion of the real polarizability in near-resonant regions of pyrimidine, the near-edge absorption fine structure (NEXAFS) of ammonia, and the direct determination of the C6 dipole-dipole dispersion coefficient of the benzene dimer.
Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules

Based on an asymmetric Lanczos-chain subspace algorithm, damped coupled cluster linear response functions have been implemented for the hierarchy of coupled cluster (CC) models including CC with single excitations (CCS), CC2, CC with single and double excitations (CCSD), and CCSD with noniterative triple corrected excitation energies CCSDR(3). This work is a first step toward the extension of these theoretical electronic structure methods of well-established high accuracy in UV-vis absorption spectroscopies to applications concerned with x-ray radiation. From the imaginary part of the linear response function, the near K-edge x-ray absorption spectra of neon, water, and carbon monoxide are determined and compared with experiment. Results at the CCSD level show relative peak intensities in good agreement with experiment with discrepancies in transition energies due to incomplete treatment of electronic relaxation and correlation that amount to 1-2 eV. With inclusion of triple excitations, errors in energetics are less than 0.9 eV and thereby capturing 90%, 95%, and 98% of the relaxation-correlation energies for C, O, and Ne, respectively.

First-order properties and Buckingham birefringence of N$_2$O and OCS – A computational (re)investigation

Prompted by recent experimental reinvestigations of the Buckingham birefringence of CO, CO$_2$, OCS and N$_2$O, we have carried out our own reinvestigation of the relevant first- and second-order properties entering the electric-field-gradient-induced birefringence effect of N$_2$O and OCS by means of state-of-the-art quantum chemical methods. The computed and experimentally derived results remain at significant variance, also in consequence of a remarkable disagreement between
the ab initio and the experimental values of the quadrupole moment relative to the centre of the nuclear masses.

General information
Publication status: Published
Organisations: University of Trieste, Università di Bologna, CNR
Contributors: Coriani, S., Puzzarini, C., Rizzo, A.
Pages: 2543-2555
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Molecular Physics
Volume: 110
Issue number: 19-20
ISSN (Print): 0026-8976
Ratings:
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.62 SJR 0.821 SNIP 0.722
Web of Science (2012): Impact factor 1.67
ISI indexed (2012): ISI indexed yes
Original language: English
DOIs:
10.1080/00268976.2012.709284
Research output: Contribution to journal › Journal article – Annual report year: 2012 › Research › peer-review

Range-dependent Adiabatic Connections
Recently, we have implemented a scheme for the calculation of the adiabatic connection linking the Kohn-Sham system to the physical, interacting system. This scheme uses a generalized Lieb functional, in which the electronic-interaction strength is varied in a simple linear fashion, keeping the potential or the density fixed in the process. In the present work, we generalize this scheme further to accommodate arbitrary two-electron operators, allowing the calculation of adiabatic connections following alternative paths as outlined by Yang [J. Chem. Phys. 109, 10107 (1998)]. Specifically, we examine the error-function and Gaussian-attenuated error-function adiabatic connections. We explore the high-density and strong static-correlation regimes for two-electron systems. The resulting adiabatic connections give an alternative view of the exchange-correlation problem and their utility for the development of new exchange-correlation functionals in Kohn-Sham and range-separated hybrid schemes is discussed.

General information
Publication status: Published
Organisations: University of Oslo, University of Trieste
Contributors: Teale, A. M., Coriani, S., Helgaker, T.
Number of pages: 8
Publication date: 2012
Peer-reviewed: Yes
DOIs:
10.1063/1.4771706
Source: FindIt
Source ID: 250075845
Research output: Contribution to conference › Paper – Annual report year: 2012 › Research › peer-review

Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations
General information
Publication status: Published
Organisations: University of Oslo, University of Trieste, Aarhus University, UiT The Arctic University of Norway
Contributors: Helgaker, T., Coriani, S., Jørgensen, P., Kristensen, K., Olsen, J., Ruud, K.
Pages: 543-631
Publication date: 2012
Peer-reviewed: Yes
Publication information
Comparison of standard and damped response formulations of magnetic circular dichroism

We apply damped response theory to the phenomenon of magnetic circular dichroism (MCD), and we investigate how the numerical instability associated with the simulation of the MCD spectrum from individually calculated A and B terms for close lying states can be remedied by the use of damped response theory. We also present a method for calculating the Faraday A term, formulated as a double residue of the quadratic response function.

Dispersion interactions in density-functional theory: An adiabatic-connection analysis

We present an analysis of the dispersion interaction energy and forces in density-functional theory from the point of view of the adiabatic connection between the Kohn-Sham non-interacting and fully interacting systems. Accurate coupled-cluster singles-doubles-perturbative-triples [CCSD(T)] densities are computed for the helium dimer and used to construct the exchange-correlation potential of Kohn-Sham theory, showing agreement with earlier results presented for the Hartree-Fock-Kohn-Sham method [M. Allen and D. J. Tozer, J. Chem. Phys. 117, 11113 (2002)]. The accuracy of the methodology utilized to determine these solutions is checked by calculation of the Hellmann-Feynman forces based on the Kohn-Sham densities, which are compared with analytic CCSD(T) forces. To ensure that this comparison is valid in a finite atomic-orbital basis set, we employ floating Gaussian basis functions throughout and all results are counterpoise corrected. The subtle charge-rearrangement effects associated with the dispersion interaction are highlighted as the origin of a large part of the dispersion force. To recover the exchange-correlation components of the interaction energy, adiabatic connections are constructed for the supermolecular system and for its constituent atoms; subtraction of the resulting adiabatic-connection curves followed by integration over the interaction strength recovers the exchange-correlation contribution relevant to the density-functional description of the dispersion interaction. The results emphasize
the long-ranged, dynamically correlated nature of the dispersion interaction between closed-shell species. An alternative adiabatic-connection path is also explored, where the electronic interactions are introduced in a manner that emphasizes the range of the electronic interactions, highlighting their purely long-ranged nature, consistent with the success of range-separated hybrid approaches in this context.

General information
Publication status: Published
Organisations: University of Oslo
Contributors: Strømsheim, M. D., Kumar, N., Coriani, S., Sagvolden, E., Teale, A. M., Helgaker, T.
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 135
Issue number: 19
ISSN (Print): 0021-9606
Ratings:
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.07 SJR 1.845 SNIP 1.231
Web of Science (2011): Impact factor 3.333
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Original language: English
DOIs:
10.1063/1.3660357
Source: FindIt
Source ID: 190796134
Research output: Contribution to journal › Journal article – Annual report year: 2011 › Research › peer-review

Spin flipping in ring-coupled-cluster-doubles theory
We report a critical analysis and comparison of a variety of random-phase-approximation (RPA) based approaches to determine the electronic ground-state energy. Interrelations between RPA variants are examined by numerical examples with particular attention paid to the role of spin-flipped excitations and the behaviour of the adiabatic-connection integrands where appropriate. In general, it is found that RPA variants that include Hartree–Fock exchange contributions are unsuitable as generally applicable methods for the determination of correlation energies. Of the remaining methods only the direct RPA and RPA with second-order screened exchange are recommended for general use.

General information
Publication status: Published
Organisations: University of Oslo, Karlsruher Institut für Technologie
Contributors: Klopper, W., Teale, A. M., Coriani, S., Bondo Pedersen, T., Helgaker, T.
Pages: 147-153
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Chemical Physics Letters
Volume: 510
Issue number: 1-3
ISSN (Print): 0009-2614
Ratings:
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.38 SJR 1.159 SNIP 0.997
Web of Science (2011): Impact factor 2.337
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Original language: English
DOIs:
10.1016/j.cplett.2011.04.101
Source: PublicationPreSubmission
Source ID: 139473662
Variational response-function formulation of vibrational circular dichroism

The atomic axial tensor (AAT) of vibrational circular dichroism is expressed as the frequency derivative at zero frequency of a linear response function for operators referencing a nuclear displacement and a magnetic field. This is used in the density matrix-based quasienergy derivative Lagrangian approach of Thorvaldsen et al. [J. Chem. Phys., 2008, 129, 214108] to express the AAT in a form where the need to solve response equations for the nuclear displacements is removed, significantly reducing the computation cost compared to existing formulations. The density matrix-based quasienergy derivative Lagrangian approach also allows us straightforwardly to use London atomic orbitals to remove the gauge-origin dependence and to account for the atomic orbitals’ dependence on the nuclear coordinates. The formalism is entirely based on atomic-orbital density and integral matrices and therefore amenable to linear scaling for sufficiently sparse matrices and given a linearly scaling response solver.

General information
Publication status: Published
Organisations: University of Trieste, UiT The Arctic University of Norway, Aarhus University
Contributors: Coriani, S., Thorvaldsen, A. J., Kristensen, K., Jørgensen, P.
Pages: 4224-4229
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 13
Issue number: 10
ISSN (Print): 1463-9076
Ratings:
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.184
Web of Science (2011): Impact factor 3.573
ISI indexed (2011): ISI indexed yes
Original language: English
DOIs: 10.1039/c0cp02230f
Source: FindIt
Source ID: 175346842

Projects:

Developing Theoretical Beamlines for Cutting-Edge Experiments
Coriani, S., PI, Department of Chemistry
01/05/2018 → 30/04/2023
Project: Research

Computational Spectroscopy In Natural sciences and Engineering (COSINE): CC, ADC and DFT protocols for magnetically induced CD spectroscopies and chiral spectroscopies of excited states
Fedotov, D., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor
Møller, K. B., Supervisor
H2020 Contract ID: 765739
01/09/2018 → 31/08/2021
Project: PhD

Computational Spectroscopy in Natural sciences and Engineering (COSINE): Coupled cluster methods for linear and non-linear X-ray spectroscopies, photoionisation, photodetachment and photoelectron spectroscopy
Moitra, T., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor
Møller, K. B., Supervisor
H2020 Contract ID: 765739
Marie Curie (EU-stipendium)
01/09/2018 → 31/08/2021
Award relations: Computational Spectroscopy in Natural sciences and Engineering (COSINE): Coupled cluster methods for linear X-ray spectroscopies, photoionisation, photodetachment and photoelectron spectroscopy
Project: PhD

Novel Response Methods for Challenging Phenomena
Lopez Vidal, M., PhD Student, Department of Chemistry
Coriani, S., Main Supervisor
Møller, K. B., Supervisor
Technical University of Denmark
15/09/2017 → 14/09/2020
Award relations: Novel Response Methods for Challenging Phenomena
Project: PhD

Atomistic Mechanisms of Functional Molecules
Abedi, M., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor
Henriksen, N. E., Supervisor
Papai, M. I., Supervisor
Coriani, S., Examiner
Gonzalez, L., Examiner
Worth, G. M. A., Examiner
Samfinansieret - Andet
01/02/2016 → 16/06/2019
Award relations: Atomistic Mechanisms of Functional Molecules
Project: PhD

Ultrafast molecular and X-ray science: Theory and simulations
Simmermacher, M., PhD Student, Department of Chemistry
Møller, K. B., Main Supervisor
Henriksen, N. E., Supervisor
Coriani, S., Examiner
Vendrell, O., Examiner
Mukamel, S., Examiner
Technical University of Denmark
01/04/2015 → 12/11/2018
Award relations: Ultrafast molecular and X-ray science: Theory and simulations
Project: PhD

Activities:

Physical Chemistry Chemical Physics (Journal)
Period: 4 Aug 2019
Sonia Coriani (Reviewer)
Department of Chemistry
Degree of recognition: International
Related journal
Physical Chemistry Chemical Physics
1463-9076
Central database
Activity: Editorial work and peer review › Peer review of manuscripts › Research

Molecular Properties and Interactions: A Wonderful Playground for a Theoretical Chemist
Period: 14 Jul 2019
Sonia Coriani (Invited speaker)
Related event

**ISTCP 2019 - 10th Triennial Congress of the International Society for Theoretical Chemical Physics**
*Period: 11 Jul 2019 → 17 Jul 2019*
*Tromsø, Norway*
Activity: Talks and presentations › Conference presentations

**ISTCP 2019 - 10th Triennial Congress of the International Society for Theoretical Chemical Physics**

**Revealing molecular secrets with theoretical beamlines**
*Period: 1 Jul 2019*
Sonia Coriani (Invited speaker)
Marta Lopez Vidal (Other)
Torsha Moitra (Other)
Daniil Fedotov (Other)
Rasmus Faber (Other)

**Related event**

**MQM 2019- 9th Molecular Quantum Mechanics Conference**
*Period: 30 Jun 2019 → 5 Jul 2019*
Heidelberg, Germany
Activity: Talks and presentations › Conference presentations

**Related event**

**MQM 2019- 9th Molecular Quantum Mechanics Conference**
*Period: 30 Jun 2019 → 5 Jul 2019*
Heidelberg, Germany
Activity: Talks and presentations › Conference presentations
Natural and magnetically induced dichroism effects by theoretical approaches
Period: 25 Jun 2019
Sonia Coriani (Invited speaker)
P. Stepánek (Other)
Rasmus Faber (Other)
Tuo Li (Other)
Danil Fedotov (Other)
Sarah Karbalaei Khani (Other)
Christof Hattig (Other)
Fabrizio Santoro (Other)
Department of Chemistry
Degree of recognition: International

Related event
CD#2019 - 17th International Conference on Chiroptical Spectroscopy
23/06/2019 → 27/06/2019
Pisa, Italy
Activity: Talks and presentations › Conference presentations

CD#2019 - 17th International Conference on Chiroptical Spectroscopy
Period: 23 Jun 2019 → 27 Jun 2019
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International

Related event
CD#2019 - 17th International Conference on Chiroptical Spectroscopy
23/06/2019 → 27/06/2019
Pisa, Italy
Activity: Attending an event › Participating in or organising a conference

6th C4 (Competence Center for Computational Chemistry) Workshop
Period: 5 Jun 2019
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International

Related event
6th C4 (Competence Center for Computational Chemistry) Workshop
05/06/2019 → 05/06/2019
Zürich, Switzerland
Activity: Attending an event › Participating in or organising a conference

Revealing molecular secrets with theoretical beamlines
Period: 5 Jun 2019
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
6th C4 (Competence Center for Computational Chemistry) Workshop
05/06/2019 → 05/06/2019
Roberto Improta  
Start date: 7 Apr 2019 → 10 Apr 2019  
Sonia Coriani (Host)  
Department of Chemistry  
Degree of recognition: International  
Activity: Hosting a guest lecturer

Journal of Chemical Theory and Computation (Journal)  
Sonia Coriani (Reviewer)  
Department of Chemistry  
Degree of recognition: International  
Related journal  
Journal of Chemical Theory and Computation  
1549-9618  
Central database  
Activity: Editorial work and peer review › Peer review of manuscripts › Research

Bruno Nunes Cabral Tenorio  
Start date: 16 Feb 2019 → 31 Mar 2019  
Sonia Coriani (Host)  
Department of Chemistry  
Degree of recognition: International  
Activity: Hosting a guest lecturer

MEthods and ALgorithms in Quantum Chemistry  
Period: 13 Dec 2018 → 15 Dec 2018  
Sonia Coriani (Participant)  
Department of Chemistry  
Degree of recognition: International  
Related event  
MEthods and ALgorithms in Quantum Chemistry : Celebrating 50 years of Theoretical Chemistry in Aarhus  
13/12/2018 → 15/12/2018  
Aarhus, Denmark  
Activity: Attending an event › Participating in or organising a conference

Theoretical Beamlines for Modern Spectroscopic Experiments  
Period: 13 Dec 2018  
Sonia Coriani (Invited speaker)  
Department of Chemistry  
Degree of recognition: International  
Related event  
MEthods and ALgorithms in Quantum Chemistry : Celebrating 50 years of Theoretical Chemistry in Aarhus  
13/12/2018 → 15/12/2018  
Aarhus, Denmark  
Activity: Talks and presentations › Conference presentations
Evaluation of an application for a position as junior research professor (junior BOFZAP)
Period: 16 Nov 2018 → 20 Dec 2018
Sonia Coriani (Advisor)
Department of Chemistry

Related external organisation

KU Leuven
Leuven, Belgium
Activity: Public and private sector consultancy › Consultancy

Coupled Cluster Methods for Local and Ultrafast Spectroscopies
Period: 24 Sep 2018
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International
Links:
https://www.ki.ku.dk/Forskning/fyschem/kjaergaard-group/molim-wg1-meeting/program/ (Program of the workshop)

Related event

Intra- and inter-molecular (atomic) interactions (a MOLIM Working Group 1 meeting)
23/09/2018 → 26/09/2018
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Intra- and inter-molecular (atomic) interactions (a MOLIM Working Group 1 meeting)
Period: 24 Sep 2018 → 26 Sep 2018
Sonia Coriani (Participant)
Department of Chemistry

Related event

Intra- and inter-molecular (atomic) interactions (a MOLIM Working Group 1 meeting)
23/09/2018 → 26/09/2018
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Journal of Chemical Physics (Journal)
Period: 9 Sep 2018
Sonia Coriani (Reviewer)
Department of Chemistry
Degree of recognition: International

Related journal

Journal of Chemical Physics
0021-9606
Central database
Activity: Editorial work and peer review › Peer review of manuscripts › Research

Journal of Chemical Theory and Computation (Journal)
Period: 3 Sep 2018
Sonia Coriani (Reviewer)
**Related journal**

**Journal of Chemical Theory and Computation**  
1549-9618  
Central database  
Activity: Editorial work and peer review › Peer review of manuscripts › Research

**Correlated electronic structure methods for local, ultrafast and magnetic-field induced spectroscopic effects**  
Period: 30 Aug 2018  
Sonia Coriani (Invited speaker)  
Department of Chemistry  
Degree of recognition: International

**Related event**

**Molecular Electronic Structure - MESM 2018**  
28/08/2018 → 31/08/2018  
Metz, France  
Activity: Talks and presentations › Conference presentations

**Molecular Electronic Structure - MESM 2018**  
Period: 28 Aug 2018 → 31 Aug 2018  
Sonia Coriani (Participant)  
Department of Chemistry  
Links:  
https://mesm.event.univ-lorraine.fr/

**Related event**

**Molecular Electronic Structure - MESM 2018**  
28/08/2018 → 31/08/2018  
Metz, France  
Activity: Attending an event › Participating in or organising a conference

**Journal of Chemical Theory and Computation (Journal)**  
Period: 15 Jul 2018  
Sonia Coriani (Reviewer)  
Department of Chemistry  
Degree of recognition: International

**Related journal**

**Journal of Chemical Theory and Computation**  
1549-9618  
Central database  
Activity: Editorial work and peer review › Peer review of manuscripts › Research

**Developing theoretical beamlines for local, ultrafast and magnetic-field induced spectroscopic effects**  
Period: 20 Jun 2018  
Sonia Coriani (Invited speaker)  
Marta Lopez Vidal (Other)  
Rasmus Faber (Other)
Department of Chemistry  
Degree of recognition: International  
Documents:  
16-icqc-abstract-lecture-coriani  
Links:  
https://icqc16.sciencesconf.org/  

Related event  
16th International Congress of Quantum Chemistry  
18/06/2018 → 23/06/2018  
Menton, France  
Activity: Talks and presentations › Conference presentations

16th International Congress of Quantum Chemistry  
Period: 18 Jun 2018 → 23 Jun 2018  
Sonia Coriani (Participant)  
Department of Chemistry  
Degree of recognition: International  
Links:  
https://icqc16.sciencesconf.org/  

Related event  
16th International Congress of Quantum Chemistry  
18/06/2018 → 23/06/2018  
Menton, France  
Activity: Attending an event › Participating in or organising a conference

Henrik Koch  
Start date: 1 Jun 2018 → 31 Aug 2018  
Sonia Coriani (Host)  
Department of Chemistry  
Degree of recognition: International  
Activity: Hosting a guest lecturer

Antonio Rizzo  
Start date: 1 May 2018 → 9 May 2018  
Sonia Coriani (Host)  
Department of Chemistry  
Degree of recognition: International  
Activity: Hosting a guest lecturer

255th ACS National Meeting & Exposition  
Period: 18 Mar 2018 → 22 Mar 2018  
Sonia Coriani (Participant)  
Department of Chemistry  
Related event  
255th ACS National Meeting & Exposition  
18/03/2018 → 22/03/2018  
New Orleans, United States  
Activity: Attending an event › Participating in or organising a conference

Sarah Karbalaei Khani  
Start date: 1 Mar 2018 → 1 May 2018
Sonia Coriani (Host)
Department of Chemistry
Degree of recognition: International
Activity: Hosting a guest lecturer

**Theoretical Chemistry Accounts (Journal)**
Period: 1 Jan 2018 → 2 Jul 2018
Sonia Coriani (Editor)
Department of Chemistry
Degree of recognition: International
Links:
https://link.springer.com/journal/214/topicalCollection/AC_bd33f9d2f726c05adc0c69e7ccc4a63c/page/1

**Related journal**

**Theoretical Chemistry Accounts**
1432-881X
Central database
Activity: Editorial work and peer review › Journal editor › Research

**Journal of Chemical Theory and Computation (Journal)**
Period: 8 Nov 2017
Sonia Coriani (Reviewer)
Department of Chemistry
Degree of recognition: International

**Related journal**

**Journal of Chemical Theory and Computation**
1549-9618
Central database
Activity: Editorial work and peer review › Peer review of manuscripts › Research

**Developing Theoretical Beamlines for Modern Experiments**
Period: 3 Nov 2017
Sonia Coriani (Invited speaker)
Department of Chemistry

**Related event**

**Fall Meeting of the Division for Theoretical Chemistry 2017 of the Danish Chemical Society**
03/11/2017 → 03/11/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Local & ultrafast spectroscopies by coupled cluster methods**
Period: 10 Oct 2017
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International
Links:
http://www.anorg.chem.uu.nl/FXS2013/FXS2017participants.htm (Link to participant list and abstracts)

**Related event**
Workshop on Fundamental Aspects of X-ray Spectroscopies
09/10/2017 → 11/10/2017
Utrecht, Netherlands
Activity: Talks and presentations › Conference presentations

Workshop on Fundamental Aspects of X-ray Spectroscopies
Period: 9 Oct 2017 → 11 Oct 2017
Sonia Coriani (Participant)

Department of Chemistry
Degree of recognition: International
Links:
http://www.anorg.chem.uu.nl/FXS2013/FXS2017.htm (Conference website)

Related event

PhD opponent
Period: 29 Sep 2017
Sonia Coriani (External examiner)

Department of Chemistry
Degree of recognition: International
Activity: Examinations and supervision › External examination

"Developing Theoretical "Beamlines" for Modern Experiments"
Period: 31 Aug 2017
Sonia Coriani (Invited speaker)

Department of Chemistry
Degree of recognition: International
Documents:
WATOC_Abstract_Coriani
Links:
http://www.watoc2017.com (Conference website)

Related event

The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists
27/08/2017 → 01/09/2017
Munich, Germany
Activity: Talks and presentations › Conference presentations

The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists
Period: 27 Aug 2017 → 1 Sep 2017
Sonia Coriani (Participant)

Department of Chemistry
Degree of recognition: International
Links:
http://www.watoc2017.com/ (Conference website)

Related event

The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists
27/08/2017 → 01/09/2017
Munich, Germany
Activity: Attending an event › Participating in or organising a conference
“Exploring local and ultrafast spectroscopic effects by ab initio methods”
Period: 24 Aug 2017
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
COST EUSPEC Workshop and School “Xtram17 - XUV time resolved advanced methods” : experiments and ab-initio modeling
23/08/2017 → 28/08/2017
Erice, Italy
Activity: Talks and presentations › Conference presentations

Petr Štěpánek
Start date: 14 Aug 2017 → 18 Aug 2017
Sonia Coriani (Host)
Department of Chemistry
Degree of recognition: International
Activity: Hosting a guest lecturer

Coupled cluster beamlines for modern experiments
Period: 3 Aug 2017
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
New Developments in Coupled Cluster Theory
31/07/2017 → 04/08/2017
Telluride, United States
Activity: Talks and presentations › Conference presentations

New Developments in Coupled Cluster Theory
Period: 31 Jul 2017 → 4 Aug 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International

Related event
New Developments in Coupled Cluster Theory
31/07/2017 → 04/08/2017
Telluride, United States
Activity: Attending an event › Participating in or organising a conference

Federica Frati
Start date: 28 Jun 2017 → 7 Jul 2017
Sonia Coriani (Host)
Department of Chemistry
Degree of recognition: International
Activity: Hosting a guest lecturer

Invited talk
Period: 22 Jun 2017
Sonia Coriani (Invited speaker)
Department of Chemistry

Related event

New Frontiers in Electron Correlation
20/06/2017 → 24/06/2017
Telluride, United States
Activity: Talks and presentations › Conference presentations

New Frontiers in Electron Correlation
Period: 20 Jun 2017 → 24 Jun 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International

Related event

New Frontiers in Electron Correlation
20/06/2017 → 24/06/2017
Telluride, United States
Activity: Attending an event › Participating in or organising a conference

International Conference: Molecular Properties and Computational Spectroscopy - from Esoteric Effects to Novel Probing Tools
Period: 10 Apr 2017 → 12 Apr 2017
Sonia Coriani (Organizer)
Department of Chemistry
Degree of recognition: International
Links:
http://mpcs17.pi.ipcf.cnr.it/ (Conference website)

Related event

International Conference: Molecular Properties and Computational Spectroscopy - from Esoteric Effects to Novel Probing Tools
09/04/2017 → 12/04/2017
Pisa, Italy
Activity: Attending an event › Participating in or organising a conference

Coupled Cluster Strategies for Core Spectroscopies of Ground and Excited States
Period: 24 Feb 2017
Sonia Coriani (Keynote speaker)
Department of Chemistry
Degree of recognition: International

Related event

The 57th Sanibel Meeting: The Theory Meeting for Theoreticians
19/02/2017 → 24/02/2017
St. St. Simons Island, GA, United States
Activity: Talks and presentations › Conference presentations

The 57th Sanibel Meeting
Period: 19 Feb 2017 → 24 Feb 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International
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