Curriculum Vitae et Studiorum
Ciro Achille Guido – Ph.D.

PERSONAL INFORMATION

COGNOME	GUIDO
NOME	CIRO ACHILLE
POSITION	TENURE TRACK PROFESSOR OF PHYSICAL CHEMISTRY
OFFICE	B262 – DISIT – UNIVERSITÀ DEL PIEMONTE ORIENTALE "A. AVOGADRO"
E-MAIL:	ciro.guido@uniupo.it

Ciro A. Guido is a tenure-track Professor of Physical Chemistry at the Dept. of Sciences, Innovation and Technology of Eastern Piedmont University "A. Avogadro", performing research in the field of theoretical Photophysics and Photochemistry.
He is the Head of the "LIMElab" unit of the Physical Chemistry's group, and the PI of the PRIN project "EnvELOP" funded by the Italian Ministry of University and Research (MUR).

The research activity is mainly (but not exclusively) focused on the development and implementation of theoretical and computational **models of optical and electronical properties in molecular and supramolecular systems also including the presence of polarizable environment using continuum and/or atomistic discrete descriptions (**solvent**,** anisotropic discrete embedding, such as a protein cavity, metal nanoparticle under plasmonic resonance, and so on).
He was the recipient of a Maria Zambrano (2021, NextGenerationEU, 1st classified) and a Beatriu de Pinos fellowships (2017 BP 00207); 2 LUMOMAT projects funding and 3 Habilitation as Associate Professor of Physical Chemistry in Italy, France and in Catalunya.

- **Education**:

2011: PhD in Chemistry (topic Quantum Chemistry) 70/70 cum laude – Scuola Normale Superiore (SNS) di Pisa (Italy).
2007: M. Sc. in Physical Chemistry 110/110 cum laude – Pisa University (Italy).
2005: B. Sc. in Chemistry 110/110 cum laude – Pisa University (Italy).

- **Citation Metrics**
  - h-index: **23** (Scopus, WoS, Scholar), citations: 1872 tot., 1698 no self-cit. (94%), 911 as first author. 33 articles, 1 book chapter, including 2 Chem. Sci., 2 JPCL, 9 JCTC, 1 Chem. Eur. J. (Cover article). Scopus author ID: 15072889800 - WoS: Ciro A. Guido - D-3533-2012

  - Talks in conferences: 16 (**6 as invited**) including 1 ACS meeting.

- **Grants and Fellowships**:

  - 19/06/2023. **PI** of PRIN2022 project "EnvELOP" funded by the Italian MUR. 216,736 €

  - 27/10/2022. F-Cur funded by Università di Siena. 35,000 €. Declined (moving to another institution).

  - 30/11/2021. Maria Zambrano Fellowship funded by NextGenerationEU. **1 classified, score 100/100**. Declined.

  - 07/09/2018. Fellowship "Beatriu de Pinos" for "outstanding postdoctoral researchers". 92,000€. funded by Marie Skłodowska-Curie Actions-COFUND. Declined

- 11/07/2017 - 10/07/2018. Co-PI of the LUMOMAT Project " Fully Consistent Polarization Response, FCPol-Resp", 60,000 €, funded by Région des Pays de la Loire (France) and EU.

- 11/07/2016 - 10/07/2017.Co-PI of the LUMOMAT Project "The Fate of Excitation Energy in solution, EE-Fate" 60,000 €, funded by Région des Pays de la Loire (France) and EU.

- 25/08/2009 – 31/07/2010: Erasmus placement for international mobility of SNS students. Visiting Ph.D. student at MSC group of Prof. C. Adamo. École Normale Superiéure de Paris and Chimie Paristech.

• **Scientific Habilitations:**
- 15/03/2021. Abilitation as Professorat Lector de l'Àmbit de Ciències de AQU de Catalunya: ID 1TQLV664H, 2a Convocatòria Lector (2020).
- 10/05/2019. Abilitation as Associate Professor of Physical Chemistry in Italy (ASN S.C. 03/A2 2019-2028
- 09/02/2018: French qualification for "fonctions Maîtres de Conferences" (Lecturer-Professor). Qualification number: 14231260035D. 2018-2022/14231260035P. 2014-2018

• **Software developed**:
- Gaussian 09 and Gaussian 16 commercial software: implementation of Vertical Excitation Method (VEM) and relative analytical gradients of energy.
- EXAT (S. Jurinovich, L. Cupellini , C. A. Guido and B. Mennucci, Università di Pisa, 2014). Distributed at: https://zenodo.org/record/4282773
- NTOBuilder (L. Cupellini, S. Caprasecca and C. A. Guido, Università di Pisa, 2018). Distributed at: https://zenodo.org/record/3948078

• **Editorial activity:**
- 07/10/2022: Review Editor of "Frontiers in Chemistry".
- 01/03/2021 - current: Topic Editor of Compounds (ISSN 2673-6918) MDPI.
- 10/10/2009 - current: referee of the peer-reviewed journals: The Journal of Physical Chemistry Letters; The Journal of Chemical Physics; Journal of Chemical Theory and Computation; The Journal of Physical Chemistry A,B,C; Journal of Computational Chemistry; Physical Chemistry Chemical Physics; Chemical Physics Letters; Journal of Molecular Structure; Theoretical Chemistry Accounts; New Journal of Chemistry; Scientific Reports; RSC Advances; Chirality.

• **Dissemination**
- 16/06/2016. International Workshop "EnLight Workshop 2016", Pisa University. Organizing Committee: B. Mennucci, C.A. Guido, S. Caprasecca, S. Jurinovich.
- 27/09/2016. "BRIGHT European Researchers' Night in Tuscany", coordinator of the theoretical chemistry stand (Mennucci's Lab).

• **Participation in international research projects:**
- 01/10/2021 - 30/11/2021. "ProID, Ultrafast Raman Technologies for Protein Identification and Sequencing" H2020-EU.1.2.1 ID:964363, € 2988513,75. Coord. IIT-Genova. Padova University (S. Corni group)

- 01/10/2020 - 30/09/2021. "TAME-Plasmons, a Theoretical chemistry Approach to tiME-resolved molecular Plasmonics", ERC-CoG-2015 - ERC Consolidator Grant project: GA 681285 2016-2021. 1,432,890 €. P.I. S. Corni (Padova University).

- 01/10/2018 - 30/09/2020. "Simulation of energy and electron transfer for molecules close to plasmonic nanostructures, PlasmoChem" MIUR, "Progetti FARE" grant number R164LZWZ4A, 2016-2020. 152,313 € P.I. S. Corni (Università di Padova, Italia).

- 01/07/2014 - 30/06/2016. Progetto "EnLight, The interplay between quantum coherence and environment in the photosynthetic electronic energy transfer and light-harvesting: a quantum chemical picture", ERC Starting Grant project: 277755 2011-2016, 1,300,000 €. PI: B Mennucci (Pisa University).

- 01/09/2012 – 19/06/2014. "Dinf DFT, Développement et implementation de Nouvelles fonctionnelles d'échange et corrélation en théorie de la fonctionnelle de la densité" ANR project. ANR 2010 BLANC n. 0425, 360,000 €. P.I. P. Cortona (École Centrale Paris) and C. Adamo (Chimie-Paristech).

- 01/05/2011 – 31/07/2012. "Advanced atomistic simulations for carbon capture and sequestration", Swiss National Science Foundation grant number 200021-132081. 294,510 CHF. P.I. W. Andreoni (EPFL).

• Track Record

- From the 1 December 2021, I spent less than 1 year as Assistant Professor at Siena University, performing research in the field of computational Photochemistry and Photobiology, collaborating with Prof. Massimo Olivucci, developing new theoretical/computational methodologies to describe the **polarization and dispersion** environment effects on the photochemistry of Rhodopsins, in a multireference (CASSCF/XMS-CASPT2) QM/MM protocol and interfaced with the automated Rhodopsin Model (ARM) recently developed in the lab.
- My work at University of Padova have been mainly focused on the reformulation of the time-dependent problem of the QM description of molecular systems in the presence of a polarizable external environment and/or metallic nanoparticles in terms of **open quantum systems** theory. By using a non-Markovian stochastic Schrödinger equation (SSE) formulation, a comprehensive picture of the electronic energies and the coupling between solute and solvent electronic dynamics is provided. This is indeed a new formulation of the coupling between QM methods and continuum solvation models which will allow **to increase the accuracy and achieve a complete description of the different timescales in ultrafast spectroscopies, for instance in molecular experiments involving plasmonic effects of metal nanoparticles.**
  Publications: *J. Chem. Phys.,* **152**, 174114 (2020); *J. Chem. Phys.,* **153**, 200901 (2020); *Phys. Chem. Chem. Phys.,* **22**, 16734 (2020). Funding: ERC TAME-Plasmon and MIUR FARE Plasmochem.
- In collaboration with the experimental group of Vincenzo Grillo at CNR-Nano Modena, we conceived a new kind of experiment that extends the technology of electron energy loss spectroscopy (EELS) to probe (supra-)molecular systems coupled to the analysis of the single components of orbital angular momentum (OAM) of the outcoming electrons: I theoretically demonstrated that this new spectroscopy provides information on **the multipolar components and even the chirality of molecular electronic transitions, superseding the usual optical spectroscopies for those cases that are problematic, such as dipole-forbidden transitions, at a very high spatial resolution.**
  Publication: *J. Chem. Theory Comput.*, **17**, 2364 (2021). Funding: ERC TAME-Plasmon and MIUR FARE Plasmochem.
- As CO-PI of two LUMOMAT projects in Nantes, I developed new QM methods to describe molecular electronic transition in solution that consider the correct solvent polarization response due to the electronic excited state of interest. In this framework, I developed and implemented a **Lagrangian formulation of the Vertical Excitation Method** (introduced during my Ph. D in collaboration with the group of **Prof. Thrular at Minnesota University**, *Chem. Sci.* **2**, 2143, 2011, **160 citations**) and **its analytical gradients**, opening the way to simulate with high accuracy emission spectra, quantum yields or dipole moments. On the same foot, in collaboration with X. Blase and I Duchemin of CNRS, we introduced, for the first time, the extension of **continuum models to the *many body perturbation theory* within the GW-BSE framework (the GW-BSE/PCM approach**).
  Publications: **101 total citations.** *Chem. Sci.* **9**, 4430 (2018); *Int. J. Quantum Chem.* **119**, e25711 (2019); *J. Chem. Theory Comput.*, **14**, 1544 (2018); *Phys. Chem. Chem. Phys*., **21**, 2307 (2019); *J. Chem Phy*s.**146**, 204106 (2017). Funding: LUMOMAT projects FCPol-Resp ed EE-Fate.
- During my postdoc for the ERC Project "EnLight" in the group of Prof. Mennucci, we developed **a QM/MM excitonic model to describe energy transfer processes in pigment-protein systems**, such as Light Harvesting complexes in plants and bacteria. The developed model was also extended to the calculation of different spectroscopies of multichromophoric systems, such as the **Excitonic Circular Dichroism (ECD) spectra in a gauge invariant formulation** and implemented in a Python software (EXAT) which allows the calculation of excitonic properties starting from results obtained through the Gaussian software (G09 and G16). These **strategies have been also coupled to a plasmonic description of metal nanorods, deeply analyzing the different radiative and non-radiative channels and the possibility of tuning the fluorescence by metal nanoparticles.**
  Publications: **309 total citations.** *J. Phys. Chem. Lett*. **9**, 6892 (2018); *J. Comput. Chem*. **39**, 279 (2017); *J. Phys. Chem. Lett*., **7**, 2189 (2016). Chem. Comm. 51, 10498 (2015); JCTC. **11**, 5782 (2015); JCTC, 9, 2209 (2013). Funding: ERC project EnLight
- The quantum mechanical description of systems based on DFT was the subject of my work at École Centrale Paris, working with Prof. Pietro Cortona and Prof. Carlo Adamo. **We proposed a new functional, PBE0-1/3, and introduced two new metrics for a quantitative description of molecular excited states.** The new hybrid functional generally improves performances in the cases of barrier heights and of CT excitations and different studies from the groups of Brédas and Galli showed the very good

performances in the description of the electronic structure of organic charge-transfer molecular crystals. PBE0-1/3 is now implemented in many quantum chemistry and solid physics codes. The two new metrics have been used to evaluate the CT character of organic chromophores, to rationalize the singlet-triplet gap in organic light-emitting diode (OLED) materials, and a relationship with the nonlinear optical properties of push-pull systems was also provided [JCTC,11,4182 (2015)]. Their definition has been also extended to tight binding TD-DFT, and implemented in an open-source code, *Multiwfn*. **On this subject we already received more than 250 citations.** Publications: **322 total citations.** *J. Chem. Phys.* **140**, 104101 (2014); *J. Chem. Theory Comput.* **9**, 3118 (2013); J. Chem. Phys. **138**, 021104 (2013). Funding: ANR project "Dinf-DFT"

- I performed ab-initio Car-Parrinello molecular dynamics simulations to study the fundamental reactions accompanying the capture of carbon dioxide in amine solutions at fully atomistic level, during my first postdoctoral experience at the Centre Européen de Calcul Atomique et Moléculaire (CECAM) in Lausanne, working with Prof. Andreoni. I investigated the role of the zwitterionic carbamate, a species long proposed as intermediate in the formation of a stable carbamate in a dilute aqueous solution. **We have shown that CO2 release and deprotonation are competitive routes for its dissociation and that water molecules play a crucial role in both pathways resulting in large entropic effects**. Publication: **40 citations** J. Chem. Theory Comput. 9, 28 (2013). Funding: Swiss National Science Foundation project n. 132081.
- Other research interests, during my PhD at **Scuola Normale Superiore di Pisa,** include the benchmarking of TDDFT performances (JPCA, 114, 13402, 2010; PCCP 12, 8016, 2010, **166 citations**) in collaboration with Prof. Carlo Adamo at Chimie-Paristech, and the implementation of a fully automated algorithm for the **anharmonic second order perturbative correction to the infrared absorption intensities** in the Gaussian suite of programs (CPL 496, 157, 2010, **103 citations**), in collaboration with Prof. V. Barone, past director of Scuola Normale.

• Selected publication:

• "Exploring the spatial features of electronic transitions in molecular and biomolecular systems by swift electrons"
C. A. Guido*, E. Rotunno, M. Zanfrognini, S. Corni and V. Grillo, *J. Chem. Theory Comput*, **17**, 2364 (2021). *Corresponding Author.

In this contribution a conceived new kind of experiment is proposed, that extends the technology of electron energy loss spectroscopy (EELS) to probe (supra-)molecular systems. Indeed, understanding the electronic structure of matter is a formidable task that largely made use of optical spectroscopies and their corresponding selection rules, but not all the electronic transitions can be probed: for instance, a long debate in the literature is still ongoing on the possible role of charge transfer (CT) states in photosynthetic mechanisms: being dark, it can only be indirectly probed. On the other hand, electron-beam spectroscopies are now emerging as probing techniques to study optical excitations with combined space, energy, and time resolution.
Performed in a scanning transmission electron microscope, EELS is based on inelastic scattering of fast electrons in a thin specimen and, very recently, new electron optics configuration has been introduced, opening the way to the analysis of the single components of orbital angular momentum (OAM) of the outcoming electrons. **Physical insight into the proposed experiment is provided by means of a rigorous model to obtain the transition rate and the selection rule.** Numerical simulations of DNA G-quadruplexes and other biomolecular systems, based on time dependent density functional theory calculations, point out that **the conceived new technique can probe the multipolar components and even the chirality of molecular transitions, superseding the usual optical spectroscopies for those cases that are problematic, such as dipole-forbidden transitions, at a very high spatial resolution.**

The work has been selected for ACSLiveSlides.

• "An Open Quantum System Theory for Polarizable Continuum Models "
C. A. Guido, M. Rosa, R. Cammi and S. Corni, *J. Chem. Phys.* 152, 174114 (2020).

In this work the time dependent (TD) problem of a solute described by Quantum Chemistry within an environment represented as a polarizable continuum model (PCM) has been reconsidered in terms of the open quantum systems (OQS) theory.
In particular, by using a non-Markovian stochastic Schrödinger equation (SSE) formulation, a comprehensive picture of the electronic energies and the coupling between solute and solvent electronic dynamics is provided: **it proves to be a unifying theoretical framework able to describe the delayed solvent response due to the solute charge density reorganization evolving in a time regime, naturally including polarization and dispersion interactions** (due to the solute fluctuations and solvent polarization response and vice versa). The **OQS-PCM accounts, by construction, for the proper coupled time scales of solute and solvent electronic dynamics and covers all the possible relative time scales of electronic solute and solvent responses**, from the limit where the solute electronic dynamics is much faster than the solvent one to the opposite limit where the solvent electronic response is considered faster than any electronic dynamics taking place in the solute.

• "Excited State Gradients for State-Specific Continuum Solvation Models: the Vertical Excitation Model within a Lagrangian TDDFT formulation"
C. A. Guido*, G. Scalmani, B. Mennucci and D. Jacquemin, J. Chem Phys.146, 204106 (2017). *Corresponding Author.

This study presents the analytical expression of the gradients of the Vertical Excitation Model approach, for which I used a Lagrangian formulation in the TD-DFT framework. The method here presented opens the way to calculate excited state (ES) properties and optimize ES molecular structures using a state-specific (SS) solvation model that represents the correct polarization response scheme.

The SS corrections become of fundamental importance for electronic transitions involving a very large electron density rearrangement. **This is the first work on ES geometry optimization by SS TDDFT analytical gradients in literature**. The method here presented can be extended to other types of polarizable response of the environment, therefore also to discrete models, such as polarizable molecular mechanics (MM) in QM/MM methods.

• "The Bethe-Salpeter formalism with polarizable continuum embedding: combining state-specific and linear-response features"
I. Duchemin, **C. A. Guido**, D. Jacquemin and X. Blase, *Chem. Sci.* **9**, 4430 (2018).

This work introduces, for **the first time, the combination of the GW and Bethe–Salpeter equation (BSE) formalism with the PCM approach.** In particular, I contribute to this work by demonstrating that **GW/BSE-PCM straightforwardly includes, on the same footing, both linear-response (LR) and state-specific (SS) contributions to the solvatochromic shifts**.
This result was established on analytic grounds as well as by comparing the numerical results obtained for several molecules or complexes using BSE + PCM or TD-DFT + PCM approaches, the latter being performed with both the LR and corrected-LR formalisms. It is important to remark that, later on, by using the framework of the open quantum system theory, I pointed out that GW-BSE/PCM can include also regimes where the solvent response is much faster than the solute electrons (see JCP, 152, 174114, 2020).

• "On the metric of charge transfer molecular excitations: a simple chemical descriptor"
C. A. Guido*, P. Cortona, B. Mennucci and C. Adamo, *J. Chem. Theory Comput.* **9**, 3118 (2013). *Corresponding Author.

In this contribution, a new index is defined with the aim of further exploring the metric of excited electronic states in the framework of the time-dependent density functional theory. This descriptor, called Δr, is based on the charge centroids of the orbitals involved in the excitations and can be interpreted in terms of the hole–electron distance. The tests carried out on a set of molecules characterized by a significant number of charge-transfer excitations well illustrate its ability in discriminating between short (Δr ≤ 1.5 Å) and long-range (Δr ≥ 2.0 Å) excitations. **Based on the well-known pitfalls of TD-DFT, its values can be then associated to the functional performances in reproducing different type of transitions and allow for the definition of a "trust radius" for GGA and hybrid functionals.** The study of some well-known difficult cases for other metric descriptors gives further evidence of **the high discrimination power of the proposed index**, **that received a very large number of citations (more than 200)** and have been implemented also in different software (G16 development versions, Multiwfn and NTOBuilder just cite few).

PUBLICATION LIST

35 publications: 34 journal articles, 1 book chapter

Citation Metrics

Web of Science (WoS): Ciro A. Guido - D-3533-2012
WoS ResearcherID: AAG-4460-2020
Scopus author ID: 15072889800
ORCID number: 0000-0003-1924-2862

h-index: **23** (Scopus, WoS, Scholar)

Times cited: **1872** from 1604 articles (Scopus).

Corresponding author (*).

- **Journal articles:**

1. **"**CPL calculations of [7]helicenes with alleged exceptional emission dissymmetry values"
   C. A. Guido*, F. Zinna and G. Pescitelli *J. Mater. Chem. C*, DOI: 10.1039/D3TC01532G (2023).
   IF: 8.067 Q1 Chemistry and Material Sciences.

2. "A Simple Protocol for Capturing both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models"
   C. A. Guido*, A. Chrayteh, G. Scalmani, B. Mennucci and D. Jacquemin *J. Chem. Theory Comput*, 17, 5155 (2021).
   IF: 6.006 Q1 Physical and Theoretical Chemistry.

3. "Exploring the spatial features of electronic transitions in molecular and biomolecular systems by swift electrons"
   C. A. Guido* E. Rotunno, M. Zanfrognini, S. Corni and V. Grillo, *J. Chem. Theory Comput*, **17**, 2364 (2021).
   IF: 6.006. Q1 Physical and Theoretical Chemistry. **Selected for ACSLiveSlides**

4. "Hybrid theoretical models for molecular nanoplasmonics".
   E. Coccia, J. Fregoni, **C. A. Guido**, M. Marsili, S. Pipolo and S. Corni J. Chem. Phys. **153**, 200901 (2020).
   IF: 3.488. Q1 Physical and Theoretical Chemistry

5. "Investigating ultrafast two-pulse experiments on single DNQDI fluorophores: a stochastic quantum approach ".
   G. Dall'Osto, E. Coccia, **C. A. Guido** and S. Corni, *Phys. Chem. Chem. Phys.* **22**, 16734 (2020).
   IF: 3.676. Q1 Physical and Theoretical Chemistry.

6. "An Open Quantum System Theory for Polarizable Continuum Models "
   C.A.Guido, M. Rosa, R. Cammi and S. Corni, *J. Chem. Phys.* 152, 174114 (2020)
   IF: 3.488. Q1 Physical and Theoretical Chemistry.

7. "On the description of the environment polarization response to electronic transitions" **Invited Perspective**.
   C. A. Guido* and S. Caprasecca, *Int. J. Quantum Chem.* **119**, e25711 (2019).
   IF: 2.444. Q1 Physical and Theoretical Chemistry.

8. "First-principles investigation of the double ESIPT process in a thiophene-based dye"
   P. Vérité, **C. A. Guido** and D. Jacquemin, *Phys. Chem. Chem. Phys*., **21**, 2307 (2019).
   IF: 3.676. Q1 Physical and Theoretical Chemistry

9. "Coupling to Charge Transfer States Is the Key to Modulate the Optical Bands for Efficient Light-Harvesting in Purple Bacteria"
   L. Cupellini, S. Caprasecca, **C. A. Guido**, F. Müh, T. Renger and B. Mennucci. J. Phys. Chem. Lett. **9**, 6892 (2018).
   IF: 6.475. : Q1 Material Science (miscellaneous)

10. "Excited State Dipole Moments in Solution: Comparison Between State-Specific and Linear-Response TD-DFT Values"
    C. A. Guido*, B. Mennucci, G. Scalmani and D. Jacquemin, *J. Chem. Theory Comput.*, **14**, 1544 (2018).

IF: 6.006. Q1 Physical and Theoretical Chemistry

11. "Density-dependent formulation of dispersion interactions in hybrid QM/MM models"
C. Curutchet, L. Cupellini, J. Kongsted, S. Corni, L. Frediani, A. Hykkerud Steindal, **C. A. Guido**, G. Scalmani, B. Mennucci, J*. Chem. Theory Comput.*, 14, 1671 (2018).
IF: 6.006. Q1 Physical and Theoretical Chemistry

12. "The Bethe-Salpeter formalism with polarizable continuum embedding: combining state-specific and linear-response features"
I. Duchemin, **C. A. Guido**, D. Jacquemin and X. Blase, *Chem. Sci.* **9**, 4430 (2018).
IF: 9.825. Q1 Chemistry.

13. "EXAT: EXcitonic Analysis Tool"
S. Jurinovich, L. Cupellini, **C. A. Guido** and B. Mennucci*, J. Comput. Chem.* **39**, 279 (2017).
IF: 3.376. Q1 Physical and Theoretical Chemistry

14. "Metrics for Molecular Electronic Excitations: A Comparison between Orbital- and Density-Based Descriptors"
M. Savarese, **C. A. Guido**, E. Brémond, I. Ciofini and C. Adamo, *J. Phys. Chem A* 121, 7543 (2017).
IF: 2.781. Q1 Physical and Theoretical Chemistry

15. "Excited State Gradients for State-Specific Continuum Solvation Models: the Vertical Excitation Model within a Lagrangian TDDFT formulation"
C. A. Guido*, G. Scalmani, B. Mennucci and D. Jacquemin, *J. Chem Phy*s. 146, 204106 (2017).
IF: 3.488. Q1 Physical and Theoretical Chemistry

16. "Control of Coherences and Optical Responses of Pigment-Protein Complexes by Plasmonic Nanoantennae."
S. Caprasecca, **C. A. Guido**, and B. Mennucci. *J. Phys. Chem. Lett*., 7, 2189 (2016).
IF: 6.475. Q1 Material Science (miscellaneous)

17. "Circularly Polarized Luminescence from Axially Chiral BODIPY DYEmers: an Experimental and Computational Study" Selected as cover article.
F. Zinna, T. Bruhn, **C. A. Guido**, J. Ahrens, M. Bröring, L. Di Bari, and G. Pescitelli. *Chem. Eur. J.* 22, 16089 (2016).
IF: 5.236. Q1 Chemistry (miscellaneous)

18. "An Ab Initio Description of the Excitonic Properties of LH2 and Their Temperature Dependence"
L. Cupellini, S. Jurinovich, M. Campetella, S. Caprasecca, **C. A. Guido**, S. M. Kelly, A. T. Gardinier, R. Cogdel, and B. Mennucci. *J. Phys. Chem. B*, 120, 11348 (2016).
IF: 2.991. Q1 Physical and Theoretical Chemistry

19. "Electronic Excitations in Solution: The Interplay between State Specific Approaches and a TD-DFT Description"
C. A. Guido*, D. Jacquemin, C. Adamo and B. Mennucci. J. Chem. Theory Comput. 11, 5782 (2015).
Top 20 monthly most read articles.
IF: 6.006. Q1 Physical and Theoretical Chemistry

20. "Negative Solvatochromism of Push-pull Biphenyl Compounds: A Theoretical Study"
S. Meng, S. Caprasecca, **C. A. Guido**, S. Jurinovich, and B. Mennucci. Theor. Chem. Acc. 134, 150 (2015).
IF: 1.702. Q2 Physical and Theoretical Chemistry

21. "Circular Dichroism and TDDFT Investigation of Chiral Fluorinated ArylBenzyl Sulfoxides"
R. Berardozzi, **C. A. Guido**, M. A. M. Capozzi, C. Cardellicchio, L. Di Bari and G. Pescitelli. Eur. J. Org. Chem. 25/2015, 5554 (2015).
IF: 3.021. Q1 Organic Chemistry

22. "The role of magnetic-electric coupling in the exciton-coupled ECD spectra. The case of bis-phenanthrenes."
S. Jurinovich, **C. A. Guido**, T. Bruhn, G. Pescitelli and B. Mennucci, Chem. Comm. 51, 10498 (2015).
IF: 6.222. Q1 Chemistry (miscellaneous)

23. "Plasmon Enhanced Light-Harvesting: Multiscale Modeling of the FMO Protein Coupled With Gold Nanoparticles".
O. Andreussi, S. Caprasecca, L. Cupellini, I. Guarnetti Prandi, **C. A. Guido**, S. Jurinovich, L. Viani, and B. Mennucci, *J. Phys. Chem. A* 119, 5197 (2015).
IF: 2.781. Q1 Physical and Theoretical Chemistry

24. "Effective Electron Displacements: a tool for TD-DFT Computational Spectroscopy"
C. A. Guido*, P. Cortona and C. Adamo, *J. Chem. Phys.* 140, 104101 (2014).
IF: 3.488. Q1 Physical and Theoretical Chemistry

25. "On the metric of charge transfer molecular excitations: a simple chemical descriptor"
C. A. Guido*, P. Cortona, B. Mennucci and C. Adamo, *J. Chem. Theory Comput.* 9, 3118 (2013).
Top 20 monthly most read articles
IF: 6.006. Q1 Physical and Theoretical Chemistry

26. "Benchmarking TD-DFT for excited state geometries of organic molecules in gas-phase and in solution"
C. A. Guido*, S. Knecht, J. Kongsted and B. Mennucci, J. Chem. Theory Comput. 9, 2209 (2013).
Top 20 monthly most read articles
IF: 6.006. Q1 Physical and Theoretical Chemistry

27. "One Third: a new recipe for the PBE0 paradigm"
C. A. Guido, E. Brémond, C. Adamo and P. Cortona J. Chem. Phys. 138, 021104 (2013).
Top 20 most read communications of 2013
IF: 3.488. Q1 Physical and Theoretical Chemistry.

28. "The Fate of a Zwitterion in Water from Ab-Initio Molecular Dynamics: Monoethanolamine (MEA)-CO2"
C. A. Guido, F. Pietrucci, G. A. Gallet and W. Andreoni, J. Chem. Theory Comput. 9, 28 (2013).
Top 20 monthly most read articles
IF: 6.006. Q1 Physical and Theoretical Chemistry

29. "Practical computation of electronic excitation in solution: vertical excitation model"
A. V. Marenich, C. J. Cramer, D. G. Truhlar, **C. A. Guido**, B. Mennucci, G. Scalmani and M. J. Frisch, Chemical Science, 2, 2143 (2011).
IF: 9.825.Q1 Chemistry

30. "On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules"
C. A. Guido*, D. Jacquemin, C. Adamo and B. Mennucci, J. Chem. Phys. A, 114, 13402 (2010).
Top 20 monthly most read articles
IF: 2.781. Q1 Physical and Theoretical Chemistry

31. "A fully automated implementation of VPT2 Infrared intensities "
V. Barone, J. Bloino, **C. A. Guido** and F. Lipparini, Chem. Phys. Lett. 496, 157 (2010).
Top 20 monthly most read articles
IF: 2.328. Q2 Physical and Theoretical Chemistry

32. "Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory"
C. A. Guido, B. Mennucci, D. Jacquemin and C. Adamo, Phys. Chem. Chem. Phys. 12, 8016 (2010).
IF: 3.676. Q1 Physical and Theoretical Chemistry

33. "Structures and properties of electronically excited chromophores in solution from the polarizable continuum model coupled to the Time-Dependent Density Functional Theory "
B. Mennucci, C. Cappelli, **C. A. Guido**, R. Cammi and J. Tomasi, J. Phys. Chem. A 113, 3009 (2009).
IF: 2.781. Q1 Physical and Theoretical Chemistry

34. "Calorimetric investigation of the aggregation of lithium perfluorooctanoate on poly(ethyleneglycol) oligomers in wate "
P. Gianni, L. Bernazzani, **C. A. Guido** and V. Mollica, THERMOCHIMICA ACTA, 451, 73 (2006).
IF: 3.115. Q2 Physical and Theoretical Chemistry

- **Book chapters:**

1. "Computational studies of environmental effects and their interplay with experiment"
B. Mennucci, S. Caprasecca and **C. A. Guido**, Advances in Physical Organic Chemistry, Volume 50, 2016, Elsevier. DOI: 10.1016/bs.apoc.2016.04.001.

Poster Communication:

1. Ciro A. Guido, Enzo Rotunno, Matteo Zanfrognini, Vincenzo Grillo, Stefano Corni
   "Simulating advanced excitation energy loss spectroscopies of molecular excitations" ISTCP-X, Tromso (Norway), 11-17 July 2019.

2. "Excited State Gradients for a State-Specific Continuum Solvation Approach: a Lagrangian TDDFT Formulation and Implementation of VEM"
   WATOC 2017, Munich (Germany), 27 August - 1 September 2017.

3. Guido Ciro Achille, Jurinovich Sandro, Loco Daniele, Pescitelli Gennaro and Mennucci Benedetta
   "*A QM excitonic scheme for simulating electronic circular dichroism spectra of multichromophoric systems*."
   International Congress of Quantum Chemistry 2015, IAQMS, Beijing (China), 8-13 June 2015.

4. Guido Ciro Achille, Cortona Pietro, Mennucci Benedetta and Adamo Carlo
   "On the metric of charge transfer molecular excitations: a simple chemical descriptor".
   DFT 2013, Durham University (U.K.), 9th -13th September 2013.

5. Guido Ciro Achille, Brémond Eric, Adamo Carlo and Cortona Pietro
   "One Third: a new recipe for the PBE0 paradigm".
   GDR CoDFT 2013, Guidel Plage (France), 21th – 24th May 2013.

6. Guido Ciro Achille, Mennucci Benedetta, Jacquemin Denis and Adamo Carlo
   "Planar versus twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory".
   Italian National Congress of Physical Chemistry, Società Chimica Italiana, Stresa (Italy), 20-24 September, 2010.

7. Guido Ciro Achille, Mennucci Benedetta, Jacquemin Denis and Adamo Carlo
   "Planar versus twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory".
   IX Girona Seminar: Electron Density, Density Matrices, and Density Functional Theory, University of Girona, Girona (Spain), 5th – 8th July 2010

8. Guido Ciro Achille, Mennucci Benedetta, Jacquemin Denis and Adamo Carlo
   "Planar versus twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory".
   Winter Modeling 2010, Scuola Normale Superiore di Pisa, Pisa (Italy), 26th February 2010

9. Guido Ciro Achille, Mennucci Benedetta and Adamo Carlo, "A systematic study of TD-DFT performance in the determination of excited state geometry and properties".
   DFT09, Université Claude Bernard Lyon 1, Lyon (France) 31th August – 4th September 2009

10. Guido Ciro Achille, Mennucci Benedetta, Cappelli Chiara, Cammi Roberto,Tomasi Jacopo,"TDDFT-IEFPCM study of electronic excited state structures and properties in solution".
    Winter Modeling '08. Pisa, 17th December 2008

11. Guido Ciro Achille, Cappelli Chiara, Mennucci Benedetta, Cammi Roberto, Tomasi Jacopo,
    "Julolidine-Malononitrile and IndolineDimethine-MalonoNitrile: a TDDFT-IEFPCM study of electronic excited state structures and properties in solution".
    XIV ESCMQC. Isola d'Elba (Italy), 8th -12th September 2008

Alessandria, 28/10/2022