Guglielmo Monaco

Curriculum Vitae et Studiorum

Personal Data

Birth	**Salerno**, *01/05/1973*.
Nationality	**Italian**.
Marital Status	**Married**, *4 children*.

Address

Office **Dipartimento di Chimica e Biologia**
Università degli Studi di Salerno
Via Giovanni Paolo II, 132
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Italy.

Internet Links

ORCID	**0000-0001-5268-940X**.
Researcher-ID	**A-6337-2008**.

Career and Titles

Apr,10 2017 –	**Habilitation for associate professorship of Physical Chemistry**, *disciplinary field 03/A2*, MIUR.
Apr,10 2017 –	**Habilitation for associate professorship of General and Inorganic Chemistry**, *disciplinary field 03/B1*, MIUR.
Apr,10 2017 –	**Habilitation for associate professorship of Fondamenti Chimici delle Tecnologie**, *disciplinary field 03/B2*, MIUR.
Oct,2 2002 –	**Assistant Professor of Physical Chemistry**, *Department of Chemistry*, University of Salerno.
1999 –2002	**Post-Doc position**, *Department of Chemistry*, University of Salerno, Prof. A. Immirzi.

Education

Feb, 2 2000 **PhD Thesis defense**, *Thesis title: "Study of heterogeneous Ziegler-Natta catalysts"*.

1996–1999 **PhD in Chemistry**, *Department of Chemistry of the University of Naples "Federico II"*, Advisor: Prof. P. Corradini. .

Jul, 19 1996 **Degree in Chemistry**, *Thesis title: "Configurational analysis of polypropylenes by high resoultion 13C NMR"* , score: 110/110 summa cum laude, Thesis advisor: Prof. V. Busico.

1991–1996 **Master in Chemistry**, *University of Naples "Federico II"* , Physical Chemistry track, mean score 29/30 on 24 exams.

1986–1991 **High School Liceo Classico "F. De Sanctis"**, *Salerno*, final score 60/60.

Publications - Edited Books

- Abbona, F.; Del Re G.; Monaco G., Eds.
  Complessità dinamica dei processi educativi. Aspetti teorici e pratici.
  320 pp. Franco Angeli (2008)
  ISBN: 9788856805543

Publications - Journal Papers

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Reversal of Clar's Aromatic?Sextet Rule in Ultrashort Single?End?Capped [5,5] Carbon Nanotubes
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65. Monaco,* G.; Tiffner, M.; Di Mola, A.; Herrebout, W.; Waser, M; Massa,* A.
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Molecules **2020**, *25*, 2272.
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64. Berger,* R. J. F.; Monaco, G.; Zanasi, R.
On the topology of total and diamagnetic induced electronic currents in molecules
J. Chem. Phys. **2020**, *19*, 194101.
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63. Monaco, G.; Summa, F. F.; Zanasi,* R.
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62. Piccardo, M.; Soncini,* A.; Fowler, P. W.; Monaco,* G.; Zanasi, R.
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61. Stanger,* A.; Monaco, G.; Zanasi,* R.
NICS-*XY*Scan Predictions of Local, Semi-Global, and Global Ring Currents in Annulated Pentalene and s-Indacene Cores Compared to First Principles Current Density Maps
ChemPhysChem **2020**, *21*, 65–82.
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60. Monaco,* G.; Procida, G.; Di Mola, A.; Herrebout, W.; Massa, A.
Error bounds on goodness of fit indicators in vibrational circular dichroism spectroscopy
Chem. Phys. Lett. **2020**, *739*, 137000.
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59. Monaco,* G.; Zanasi, R.
Delocalization energy retrieved from the current density tensor
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58. Monaco, G; Zanasi,* R.
Magnetically Induced Current Density Spatial Domains
J. Phys. Chem. A **2019**, *123*, 1558-1569.
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57. Monaco,* G; Zanasi, R.
Field-independent current strength
Theor. Chem. Acc. **2018**, *137*, 103.
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56. Monaco,* G; Zanasi,* R.
AACID: Anisotropy of the Asymmetric Magnetically Induced Current Density Tensor
J. Phys. Chem. A **2018**, *122*, 4681–4686.
doi:10.1021/acs.jpca.8b03663

55. Monaco,* G; Zanasi,* R.
Analysis of the Nucleus-Independent Chemical Shifts of [10]Cyclophenacene: Is It an Aromatic or Antiaromatic Molecule?
J. Phys. Chem. Lett. **2017**, 4673–4678.
doi:10.1021/acs.jpclett.7b0193

54. Monaco, G.; Fedullo, A.
Teaching Least Squares in Matrix Notation
Ratio Mathematica **2017**, *32*, 63-75.
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53. Monaco,* G; Aquino, F; Zanasi, R; Herrebout, W; Bultinck, P; Massa, A.
Model-averaging of ab initio spectra for the absolute configuration assignment via vibrational circular dichroism
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52. Massa,* A; Rizzo,* P.; Scorzelli, F.; Monaco, G.; Zanasi,* R.
Determination of the absolute configuration of a novel tetrasubstituted isoindolinone by vibrational circular dichroism
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51. Concilio, G.; Talotta, C.; Gaeta, C.; Neri,* P.; Monaco,* G.; Zanasi, R.; Tedesco,* D.; Bertucci, C.
Absolute configuration assignment of chiral resorcin[4]arenes from ECD spectra
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The intriguing class of $altan$-molecules
J. Phys. Org. Chem. **2016**, *29*, 793-798.
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Inorg. Chim. Acta **2016**, *444*, 202–208.
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47. Di Mola, A.; Scorzelli, F.; Monaco, G.; Palombi, L.; Massa, A.
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RSC Adv. **2016**, *6*, 60780-60786.
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46. Meninno, S.; Rizzo, P.; Abbate, S.; Longhi, G.; Mazzeo, G.; Monaco, G.; Lattanzi,* A.; Zanasi,* R.
Absolute Configuration Assignment of a Paraconic Acid Derivative via Vibrational Circular Dichroism Spectroscopy and Density Functional Theory Calculation: Absolute Configuration Assignment of a Paraconic Acid Derivative
Chirality **2016**, *28*, 110–115.
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45. Monaco, G.
On the diatropic perimeter of iterated *altan*-molecules
Phys. Chem. Chem. Phys. **2015**, *43*, 28544–28547.
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44. Della Porta, P.; Zanasi, R.; Monaco,* G.
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J. Comp. Chem. **2015**, *36*, 707–716.
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43. Monaco, G.; Della Porta, P.; Jabłoński, M.; Zanasi,* R.
Topology of the magnetically induced current density and proton magnetic shielding in hydrogen bonded systems
Phys. Chem. Chem. Phys. **2015**, 17, 5966–5972.
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Cationic Half-Sandwich Quinolinophaneoxazoline-Based (h6-p-Cymene)ruthenium(II) Complexes Exhibiting Different Chirality Types: Synthesis, and Structural Determination by Complementary Spectroscopic Methods.
Dalton Transactions **2014**, *43*, 1636.
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41. Pelloni,* S.; Monaco,* G.; Della Porta, P.; Zanasi, R.; Lazzeretti, P.
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J. Phys. Chem. A **2014**, *118*, 3367–3375.
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40. Monaco,* G.; Zanasi, R.
Assessment of Ring Current Models for Monocycles
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39. Monaco*, G.; Zanasi, R.
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36. Jabłoński*, M., Monaco*, G.
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Org. Biomol. Chem. **2012**
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32. Monaco,* G., Zanasi, R.
Three Contra-Rotating Currents from a Rational Design of Polycyclic Aromatic Hydrocarbons: *altan*-Corannulene and *altan*-Coronene.
J. Phys. Chem. A **2012**, *116*, 9020–9026.
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31. Monaco, G.; Zanasi, R.
Searching for a good candidate to perform a chiral nuclear magnetic field resonance experiment in disordered phase: a study of 8,9-difluoro-P-hexahelicene.
Chirality **2011**, *23*, 752- 755.
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30. Pelloni, S.*; Monaco, G.*; Lazzeretti, P.; Zanasi, R.
Beyond NICS: estimation of the magnetotropicity of inorganic unsaturated planar rings.
Phys. Chem. Chem. Phys. **2011**, *13*, 20666-20672.
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29. Monaco, G.
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28. Pelloni, S.; Lazzeretti, P.*; Monaco, G.; Zanasi, R.
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Rend. Fis. Acc. Lincei **2011**,*22*, 105–112.
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27. Monaco, G; Zanasi, R.*; Pelloni, S.; Lazzeretti, P.
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Absolute Configuration Assignment of Inherently Chiral Calix[4]arenes using DFT Calculations of Chiroptical Properties.
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24. Lattanzi, A.; Russo, A.; Rizzo, P.; Monaco, G.; Zanasi, R.*
Absolute Configuration Assignment of (3-Phenyloxirane-2,2-diyl)bisPhenylmethanone via Density Functional Calculations of Optical Rotation and Vibrational Circular Dichroism.
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23. Caruso, T.; Donnamaria, C.; Artillo, A.; Peluso, A.; Spinella, A.*; Monaco, G.*
On the influence of unsaturation on the macrolactonization of hydroxy fatty acids
J. Phys. Org. Chem. **2009**, *22*, 978-985.
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On the additivity of current density in polycyclic aromatic hydrocarbons
*J. Chem. Phys.***2009**,*131*, 044126-1, 044126-10.
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On the analysis of some orbital contributions to the current density in circulenes
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20. Monaco, G., Scott, L. T., Zanasi, R.
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19. Monaco, G.
Interiorità ed educazione
Riv. giur. scuola **2007**, *46*, 215-218.
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18. Monaco, G., Fowler, P., Lillington, M., Zanasi, R.
Designing Paramagnetic Circulenes
Angew. Chem. Int. Ed. **2007**, *46*, 1189–1192.
doi: 10.1002/anie.200604261

17. Monaco*, G.;
Il cammino dello scienziato e il mito della caverna
Filosofia Oggi **2006**, *29*, 9-12
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16. Monaco*, G.; Sessa, I.; Zambelli, A.
Simple Trends in the Methylene Regions of the NMR Spectrum of Poly(propylene) and Ethylene-Propylene Copolymers

Macromol. Chem. Phys. **2006**,*207*, 1038-1048.
doi: 10.1002/macp.200600091

15. Monaco, G., Viglione, R. G., Zanasi, R., Fowler, P. W.
Designing Ring-Current Patterns: [10,5]-Coronene, a Circulene with Inverted Rim and Hub Currents.
J. Phys. Chem. A **2006** *110*, 7447-7452.
doi: 10.1021/jp0600559

14. Fedullo, A.; Antinucci, S.; Immirzi, A.; Monaco*, G.
Profile functions in diffraction patterns of semicrystalline fibers with Gaussian misalignment.
J. Macromol. Sci. B, Physics, **2005**, *44*, 1–16.
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13. Immirzi*, A.; Tedesco, C.; Monaco, G.; Tonelli, A. E.
Crystal Structure and Melting Entropy of Natural Rubber.
Macromolecules **2005**, *38*, 1223-1231.

12. Monaco*, G.; Zambelli, A. Simple trends in NMR spectra of vinyl polymers: the ^{1}H NMR spectrum of poly(propylene).
Macromol. Chem. Phys. **2005**, *206*, 203-209.

11. Caruso, T.; Monaco, G.; Peluso*, A.; Spinella*, A.
Temperature regiocontrol of intramolecular cyclization of di-hydroxysecoacids.
Org. & Biomol. Chem. **2004**, 2, 3425-3426.

10. Monaco*, G.; Viglione, Rosario G.
Simple trends in the methylene and α-substituent regions of NMR spectra of vinyl polymers.
Macromol. Chem. Phys. **2004**, *205*, 1327-1337.

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J. Polym. Sci. **2002**, *40*, 3249-3255.

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On the Microstructural Analysis of (Pseudo)copolymers
Macromol. Theory Simul. **2002**, *11*, 84-92.

7. Antinucci, S.; Monaco, G.; Immirzi*, A.
An Unusual Chain Conformation: *s*(6*4/3) Helices in Form II of Isotactic Poly(vinylcyclopentane).
Macromolecules **2001,** *34,* 8078-8083.

6. Monaco*, G.
On the Connection between Microstructure and Kinetics of (Pseudo)copolymerization
Macromolecules **2001,** *34,* 4406-4415; Correction: *Macromolecules* **2001,** *34,* 5730.
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5. Monaco, G.; Toto, M. ; Guerra, G.; Corradini, P.; Cavallo*, L.
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$MgCl_2$ Support of the Heterogeneous Ziegler-Natta Catalysts.
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4. Busico*, V.; Cipullo, R.; Monaco, G.; Talarico, G.; Vacatello, M.; Chadwick, J.C.; Segre A.L.; Sudmeijer, O.
High-resolution ^{13}C NMR configurational analysis of polypropylene made with $MgCl_2$-supported Ziegler-Natta catalysts, 1 - The <<model>> system $MgCl_2/TiCl_4$- 2,6-dimethyl-pyridine/$Al(C_2H_5)_3$.
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Macromolecules **1998**, *31*, 8713-8719.
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On the definition of the atomic charge. Relationship between ^{13}C NMR chemical shifts, dipole moments and charges in saturated hydrocarbons.
Int. J. Quantum Chem. **1998**, *31*, 201-10.
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1. Busico*, V.; Cipullo, R.; Monaco, G.; Vacatello, M.; Segre, A.L.
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Publications - Book Chapters

10. Monaco, G.
Sull'ontologia dei modelli molecolari
In *Sul valore conoscitivo dei modelli. Un contributo in scienza, filosofia e teologia*
Aracne Ed. 2017, pp.143-158. ISBN:9788825506709

9. Monaco, G.
Limitazioni del Biodeterminismo
In *La natura umana. Riflessioni transdisciplinari del gruppo Quid est veritas*;
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Beyond NICS
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Proceedings of the Conference *Theory and Applications in Computational Chemistry: the first decade of the second millennium*, Pavia, Sept 2-7, 2012;
Clementi, E.; André, J.M.; McCammon, J. A., Eds.
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7. Monaco, G.
   From Chemical Kinetics to Models of Acquisition of Information: On the Importance of the Rate of Acquisition of Information.
   In *Decision Theory and Choices: a Complexity Approach*, Faggini, M.; Vinci, C. P., Eds.; Spinger-Verlag, 2010, p. 171-182.
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6. Monaco, G.*; Zanasi, R.*
   Quantitative Indicators of Bond Current Susceptibility
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   Hersonissos, Crete (Greece), 25–30 Sept, 2008;
   Simos, T. E.; G. Maroulis, G. Eds.
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5. Monaco, G.
   Sulla possibilità di sviluppare modelli di apprendimento basati su agenti.
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   Abbona, F.; Del Re G.; Monaco G., Eds. p. 285-305, Franco Angeli (2008)
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4. Monaco, G.
   Considerazioni sulla valutazione scolastica.
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3. Monaco, G.; Zanasi, R.
   Analysis of Some Orbital Contributions to the Current Density in Circulenes.
   AIP Conf. Proc. **2007**, *963*(2), 1302-1305.
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   Corfu (Greece), 25–30 Sept, 2007
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   Proton Assisted Electron Transfer
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1. Busico*, V.; Cipullo, R.; Monaco, G.; Talarico, G.; Vacatello, M.; Chadwick, J.C.; Segre A.L.; Sudmeijer, O.
   New Insight into Propene Polymerization Promoted by Heterogeneous Ziegler-Natta Catalysts.

In *Metalorganic Catalysts for Synthesis and Polymerization*;
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Talks

20. (invited) G. Monaco,* R. Zanasi
Magnetic indicators of aromaticity,
Aromaticity 2018,
MAGIC2018
Riviera Maya (Mexico), 28 Nov-1 Dec 2018

19. (invited) G. Monaco,* R. Zanasi
AACID: the Anisotropy of the Asymmetric magnetically Induced Current Density tensor,
MAGIC2018
Kragujevac (Serbia), 23-28 Sept 2018

18. (invited) G. Monaco,* G. Procida, A. Massa, W. Herrebout
Model-averaging of ab initio spectra in vibrational spectroscopy,
VOA-6 Conference
Brescia, 9-13 Sept 2018

17. G. Monaco,* F. Aquino, R. Zanasi, W. Herrebout, A. Massa
Configuration Assignment of two Hybrid Isoindolinone-phthalide Molecules by Vibrational Circular Dichroism,
XXVI Congresso SCI
Paestum, 10-14 Sept 2017

16. G. Monaco,*
Models for the current density,
Workshop on MAGnetically Induced Current density
Salerno, 5-9 Sept 2016

15. G. Monaco,*
The intriguing class of $altan-$molecules,
European Symposium on Organic Reactivity ESOR 2015
Keil, 30 Aug-4 Sept 2015

14. (invited) G. Monaco,*
On the Chemical Meaning of the Current Density,
Workshop on Magnetically Induced Current Density
Tvärminne (Finland), 17-21 Nov 2014

13. G. Monaco,* R. Zanasi,
Ab Initio Models of Ring Current Models,
XXV Congresso SCI
Arcavacata di Rende, 7-12 Settembre 2014

12. G. Monaco,* R. Zanasi,
The unusual current density patterns of altan-molecules,
XLI Congresso Nazionale di Chimica Fisica, Alessandria, 23-27 giugno 2013.

11. G. Monaco,* R. Zanasi,
Structural Insight from the Current Density,
Gordon Research Conference on Electron Distribution & Chemical Bonding,
Les Diablerets (Svizzera), 2-7 giugno 2013.

10. G. Monaco,* R. Zanasi,
Novel Virtual Polycyclics with Unprecedented Patterns of Ring Currents,
XIII European Symposium on Organic Reactivity, Tartu, Estonia, 11-16 settembre 2011.

9. G. Monaco,*
On the Optimal Rate for the Acquisition of Information,
Decision Theory and Choice: a Complexity Approach
Salerno, June 19-20 2008

8. G. Monaco,* R. Zanasi,
Quantitative Indicators of Bond Current Susceptibility,
International Conference on Computational Methods in Science and Engineering 2008, Hersonissos, Creta, 25-30 settembre 2008.

7. G. Monaco,* R. Zanasi, Analysis of Some Orbital Contributions to the Current Density in Circulenes, International Conference on Computational Methods in Science and Engineering 2007, Corfù, 25-30 settembre 2007.

6. G. Monaco,* R. Zanasi, From Paratropic Ring Currents to closed-shell molecular paramagnets, XXXVI Congresso Nazionale di Chimica Fisica, 17-22 giugno 2007, Gallipoli.

5. (invited) G. Monaco,* Mathematical models of a school system, E-CAS WORKSHOP on Complexity and performance of educational systems, Frascati, Villa Falconieri 13-15 dicembre 2006

4. S. Antinucci, A. Immirzi, G. Monaco,* Uso di funzioni di profilo non empiriche per la valutazione delle intensità diffratte integrate, presentazione orale alle "Giornate del CIMCF - Centro Interdipartimentale di Metodologie Chimico Fisiche", Napoli, 4-5 luglio 2002.

3. (invited) G. Monaco,* Vecchie e nuove metodologie di analisi dati per la soluzione di complessi problemi strutturali seminario discusso il 21 settembre 2001 nell'ambito della III scuola nazionale di diffrazione tenutasi all'Università "La Sapienza", Roma, settembre 2001.

2. G. Monaco,* Establishing the connection between microstructural data and kinetic constants of (pseudo)copolymerization; III Workshop on "Advances on Insertion Polymerisation", Ischia, 11-13 settembre 2000.

1. G. Monaco,* Caratterizzazione 13C NMR ad alta risoluzione di polimeri vinilici: metodologia. Incontri di Risonanza Magnetica; Napoli, 30 giugno 1999.

Seminars

3. (invited) G. Monaco,*
The Magnetic Response as a Tool for Design and Classification of Aromatic Molecules,
Institute of Organic Chemistry,
Polish Academy of Sciences, Warsaw
25 Apr 2019

2. (invited) G. Monaco,* Diffrazione di materiali fibrosi seminario discusso il 17 settembre 2003 nell'ambito della V scuola sperimentale di diffrazione tenutasi all'Università "La Sapienza", Roma, settembre 2003.

1. (invited) G. Monaco,* Vecchie e nuove metodologie di analisi dati per la soluzione di complessi problemi strutturali seminario discusso il 13 settembre 2000 nell'ambito della II scuola nazionale di diffrazione tenutasi all'Università "La Sapienza", Roma, 4-16 settembre 2000.

Posters

29. Zanasi, R.; Monaco, G.
[10]Cyclophenacene: one more case of NICS failure
XXVI Congresso SCI
Paestum,10-14 Sep 2017

28. Soncini, A.; Piccardo, M.; Fowler, P. W.; Zanasi, R.; Monaco, G.
Current Density Patterns and Ground State Nature of *altan*-[n]annulenes
ISRIUM 2017
Sorrento, 18-22 June 2017

27. Zanasi, R.; Monaco, G.
[10]Cyclophenacene: one more case of NICS failure Molecular Properties and Computational Spectroscopy
Pisa,10-12 Apr 2017

26. Aquino, F; Zanasi, R.; Herrebout, W.; Massa, A.; Monaco, G.
Absolute Configuration Assignment of two Hybrid Isoindolinone-phthalide Molecules by Vibrational Circular Dichroism Molecular Properties and Computational Spectroscopy
Pisa,10-12 Apr 2017

25. Della Porta, P.; Zanasi, R.; Monaco, G.
Insights on weak bonding from the current density
European Symposium on Organic Reactivity ESOR 2015
Keil, 30 Aug-4 Sept 2015

24. Monaco, G; Tedesco, D; Zanasi, R; Concilio, G; Talotta, C; Gaeta, C; Neri, P;
Absolute Configuration Assignment of Inherently Chiral Resorcin[4]arenes
13th International Conference on Calixarenes Giardini Naxos (Messina), Italy, 5-9 Jul 2015

23. Tedesco,* D.; Přecechtělová, M; Monaco, Gaeta, C.; Talotta, C.; Concilio, G.; Neri, P.; Zanasi, R.; Bertucci, C.
Development of stopped-flow enantioselective HPLC-CD methods: Towards the stereochemical

characterization of C-undecylresorcin[4]arenes
Recent Developments in Pharmaceutical Analysis, Perugia, 28 Jun-01 Jul 2015

22. Monaco,* G.; Della Porta, P.; Zanasi, R.
H–H bonding in biphenyl: the current density perspective
Workshop on Magnetically Induced Currents in Molecules
Tvarminne (Finland), 17-21 Nov 2014

21. Monaco, G.; Tedesco, D; Talotta, C.; Gaeta, C.; Bertucci, C.; Neri, P. Absolute configuration assignment of inherently chiral resorcin[4]arenes ChirItaly 2014, Pisa, 18-20 June 2014.

20. Massa, A.; Rizzo, P.; Monaco, G. Zanasi,* R. Absolute configuration assignment made easier by the VCD of coupled oscillating carbonyls ChirItaly 2014, Pisa, 18-20 June 2014.

19. S. Superchi*, R. Ruzziconi, R. Zanasi, G. Bellachioma, G. Ciancaleoni, G. Monaco, *Sterochemistry of Quinolinophanoxazoline(η^6-p-Cimene) Ru(II) Complexes by ECD Studies* 40th International Conference on Coordination Chemistry (40ICCC) Valencia, Spain 9-13 settembre 2012.

18. R. Zanasi,* G. Longhi, S. Abbate, S. Superchi L. Pisani, A. Summa, G. Monaco Dinaphthoazepines a Vibrational Circular Dichroism Study
Vibrational Optical Activity: Interplay of Theory and Experiment September 23-27, 2012 Scuola Normale Superiore, Pisa, Italy

17. S. Superchi*, R. Ruzziconi, R. Zanasi, G. Bellachioma, G. Ciancaleoni, G. Monaco, *Sterochemistry of Quinolinophanoxazoline(η^6-p-Cimene) Ru(II) Complexes by ECD Studies* 40th Internationalk Conference on Coordination Chemistry (40ICCC) Valencia, Spain 9-13 settembre 2012.

16. G. Monaco,* R. Zanasi
How to increase the role of the perimeter in polycyclic aromatic hydrocarbons?
International Symposium on Reactive Intermediates and Unusual Molecules (ISRIUM) July 8-13, 2012 Centro Stefano Franscini, Ascona, Switzerland

15. G. Monaco A short cut to introduce the ergodic principle teaching collision theory

    Faraday Discussion 157, Assisi, 8-13 giugno 2012.

14. G. Monaco,* R. Zanasi, R. Carion, B. Champagne, S. Pelloni, P. Lazzaretti Novel insight in the magnetic tensors of cyclopropane

    IX Girona Seminar, Girona, 5-8 july 2010

13. Talotta C,* Gaeta C, Troisi F, Rizzo P, Monaco G, Zanasi R., Mazzeo G, Rosini C, Neri P *Absolute Configuration Assignment of Inherently Absolute Configuration Assignment of Inherently Chiral Meta-Substituted Calix[4]arenas Using DFT Calculations of Chiroptical Properties.*
In: IX Congresso Nazionale di Chimica Supramolecolare- atti del convegno. Parma, 6-9 Settembre 2009.

12. Gaeta C.,* Talotta C, Troisi F., Rizzo P., Monaco G., Zanasi R., Mazzeo G., Rosini, Neri P. *Absolute Configuration Assignment of Inherently Chiral Meta-Substituted Calix[4]arenas Using DFT Calculations of Chiroptical Properties*. In: 10th International Conference on Calixarenes-Proceedings. SEUL, S.Korea, July 13-16, 2009.

11. G. Monaco,* R. Zanasi,
On the Additivity of Current Density in Polycyclic Conjugated Hydrocarbons
Molecular Properties '09
Oslo, 18-21 giugno 2009.

10. G. Monaco,* R. Zanasi, *Magnetic Euripi in Corannulene*, V European Charge Density Meeting Gravedona (CO) 8-11 giugno 2008.

9. G. Monaco,* R. Zanasi,
Two useful theorems on Kasteleyn Kekulé counting
Faraday Discussion 135: Chemical Concepts from Quantum Mechanics
University of Manchester, 4-6 settembre 2006.

8. G. Monaco,* R. Zanasi, P. W. Fowler,
Designing paramagnetic coronenes
Faraday Discussion 135: Chemical Concepts from Quantum Mechanics
University of Manchester, 4-6 settembre 2006.

7. Sessa, A. Zambelli, G. Monaco,*
Sintesi e caratterizzazione di composti modello per lo studio di sequenze regioirregolari PEP in copolimeri etilene-propilene,
XVII Convegno Nazionale dell'Associazione Italiana di Scienza e Tecnologia delle Macromolecole Napoli 11-15 settembre 2005.

6. G. Monaco,* M. Causà,
Looking for a novel interpretation of the low melting entropy of natural rubber, XVII Convegno Nazionale dell'Associazione Italiana di Scienza e Tecnologia delle Macromolecole Napoli 11-15 settembre 2005.

5. A. Immirzi, C. Tedesco, G. Monaco,
Using internal coordinates studying fibrous structures, XX Congress of the International Union of Crystallography, Firenze, 23 - 31 Agosto 2005.

4. G. Monaco,* A. Zambelli
Childrens' wireless telephone game and NMR spectra of vinyl polymers
XXXIII Congresso Nazionale della Divisione di Chimica Fisica
Napoli, 21-25 Giugno 2004.

3. Caruso, T.; Monaco,* G.; Peluso, A.; Spinella, *A.*
Temperature regiocontrol of intramolecular cyclization of di-hydroxysecoacids
XXXIII Congresso Nazionale della Divisione di Chimica Fisica, Napoli, 21-25 Giugno 2004.

2. S. Antinucci, A. Immirzi, G. Monaco,*
FIDIA'S: an improved method of integration of Bragg reflections of fibrous semicrystalline materials
12th ESRF Users' Meeting – Satellite Workshop on Fibers and Polymers
Grenoble, 11-12 febbraio 2002.

1. S. Antinucci,* G. Monaco, A. Immirzi,
Un'insolita conformazione di catena: eliche 12_3 nella forma II del poli(vinilciclopentano)

XV convegno italiano di scienza e tecnologia delle macromolecole
Trieste, 24-27 settembre 2001.

Awards

Error Bounds AIE + hot paper
Model Averaging hot paper
PCCP hot paper
JCP Editor's Choice

Conference Organization

6-10 Sept. 2020 **MAGIC 2020 Workshop**, *Peterhouse*, Cambridge, Member of the Scientific Committee.
Canceled for COVID-19

5-9 Sept. 2016 **MAGIC 2016 Workshop**, *Dipartimento di Chimica e Biologia*, Salerno, President of the MAGIC2016 Local Committee.

Teaching

2008–2018 **Lecturer of Fundamental Courses:**, *Dipartimento di Chimica e Biologia*, Salerno.

- I sem. 2019-2020: Meccanica Quantistica Molecolare – modulo 2 (5 CFU)
- I sem. 2018-2019: Meccanica Quantistica Molecolare – modulo 2 (5 CFU)
- I sem. 2017-2018: Meccanica Quantistica Molecolare – modulo 2 (5 CFU)
- I sem. 2016-2017: Chimica Fisica Superiore – modulo 2 (5 CFU)
- I sem. 2015-2016: Chimica Fisica Superiore – modulo 2 (5 CFU)
- I sem. 2014-2015: Chimica Fisica Superiore – modulo 2 (5 CFU)
- I sem. 2013-2014: Chimica Fisica Superiore – modulo 2 (5 CFU)
- I sem. 2012-2013: Chimica Fisica Superiore – modulo 2 (5 CFU)
- II sem. 2011-2012: Cinetica Chimica e Dinamica Molecolare (4 CFU)
- II sem. 2011-2012: Laboratorio di Chimica Fisica I (1 CFU)
- II sem. 2010-2011: Cinetica Chimica e Dinamica Molecolare – modulo 2 (2CFU)
- II sem. 2010-2011: Laboratorio di Chimica Fisica I (3 CFU)
- II sem. 2009-2010: Cinetica Chimica e Dinamica Molecolare – modulo 2 (2CFU)
- II sem. 2009-2010: Laboratorio di Chimica Fisica I (3 CFU)
- I sem. 2009-2010: Laboratorio di Chimica Fisica II (3 CFU)
- II sem. 2008-2009: Cinetica Chimica e Dinamica Molecolare – modulo 2 (2CFU)
- II sem. 2008-2009: Laboratorio di Chimica Fisica I (3 CFU)
- II sem. 2007-2008: Cinetica Chimica e Dinamica Molecolare – modulo 2 (2CFU)
- II sem. 2007-2008: Laboratorio di Chimica Fisica I (3 CFU)
- II sem. 2006-2007: Laboratorio di Chimica Fisica I (3 CFU)
- II sem. 2005-2006: Laboratorio di Chimica Fisica I (3 CFU)

- I sem. 2004-2005: Laboratorio di Chimica Fisica II (2 CFU)
- II sem. 2003-2004: Laboratorio di Fondamenti di Elettromagnetismo (2 CFU)
- I sem. 2003-2004: Laboratorio di Chimica Fisica II (2 CFU)
- I sem. 2003-2004: Laboratorio di Chimica Analitica Quantitativa (3 CFU)
- I sem. 2002-2003: Laboratorio di Chimica Fisica I (2 CFU)

2008–2013 **Member of the PhD Evaluation Commitee**, *Dipartimento di Chimica*, Salerno.

2014 **Teacher**, *Introduction to the Scientific Method for College Students*, MIUR.

Institutional Appointments

2013–2018 **Responsible of the Process Quality**, *Chemistry Degree at the Department of Chemistry*, University of Salerno.

Referrals

2014 **Projects**, *Post-Doc project*, CINECA.

2016 **Project**, *Research proposal*, Polish National Science Centre.

2002– **Manuscripts**, *Referee for manuscripts submitted to: Chirality, Crystal Engineering Communications, Journal of Biophysical Chemistry, Journal of Physical Chemistry A, Macromolecules, Organic & Biomolecular Chemistry, Scientific Reports, Theoretical Chemistry Accounts, WIRES*.

Partecipation to National Research Projects

PRIN 2008
Sviluppo e applicazione di metodi teorici per l'assegnamento della configurazione assoluta molecolare.
Coordinatore scientifico: SCAFATO Patrizia
Responsabile scientifico: ZANASI Riccardo
Università degli Studi di SALERNO

PRIN 2004
Polimerizzazioni per la produzione di materiali elastomerici e polimerizzazioni "viventi" catalizzate da complessi metallorganici.
Coordinatore scientifico: GUERRA Gaetano
Responsabile scientifico: GUERRA Gaetano
Università degli Studi di SALERNO

PRIN 2002
Sintesi e caratterizzazione di nuovi catalizzatori di polimerizzazione e di nuovi materiali polimerici idrocarburici.
Coordinatore scientifico: GUERRA Gaetano
Responsabile scientifico: GUERRA Gaetano
Università degli Studi di SALERNO

Collaborations

In the last 5 years some works have been done in collaboration with local, national, and international groups:

A. Lattanzi	Università di Salerno
A. Massa	Università di Salerno
P. Neri	Università di Salerno
S. Abbate	Università di Brescia
P. Bultinck	University of Ghent, Belgium
W. Herrebout	University of Antwerp, Belgium
M. Jabłoński	Kepler University of Toruń, Poland

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Research Profile Sketch

Guglielmo Monaco obtained the degree in Chemistry (full marks summa cum laude, mean score 29/30 on 24 exams) by the University of Naples in 1996, discussing a thesis titled "Configurational analysis of polypropylenes by high resoultion ^{13}C NMR", with advisor Prof. V. Busico. That work required the combination of the analysis of experimental data with empirical and ab initio calculations, which were performed under the advice of Prof. G. Del Re. In 1999 a similar combination of expertise was disclosed in the doctoral thesis titled "Study of heterogeneous Ziegler-Natta catalysts", with advisor Prof. P. Corradini. He was then called by Prof. A. Immirzi at the University of Salerno for a post-doc position on the study of fibrous polymers.
Among his contribution in this first period, there is the rationalization of NMR spectra of (co)polymers (3, 10, 12, 16), a general interpretation of microstructure in terms of polymerization kinetics (6), the development of equations for the effect of misalignment on the diffraction patterns of fibrous polymers (14), the interpretation of the yields of competitive macrocyclization pathways (23).
In the last ten years his scientific activity has been mainly focused on the current density induced in closed-shell molecules by an external magnetic field. Among his contributions on this topic there is the generalization of the spectral rules for the interpretation of the current density within the CTOCD-DZ method (21), the interpretation of critical points of the current density and a corollary to Kasteleyn theorem (22), the development of aromaticity indicators for monocycles which are preferable to the widespread NICS (30), the introduction of $altan-$molecules (34).
A further activity has been the investigation of the complexity approach in education, for which we worked for INValSI to contribute to a workshop in Villa Falconieri (December 2006) and to perform an editorial review on a multidisciplinary book on complexity and education, published by Franco Angeli in 2008. A further book chapter in a Springer book is also devoted to that matter (B4).