CURRICULUM VITAE ET STUDIORUM: Dr. Francesco MUNIZ-MIRANDA

Age: 39 y.o.
Present Position: Researcher in Physical Chemistry
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EDUCATION

- **April 2007** Bachelor Degree in Chemistry (full marks) at the University of Florence (Italy) with a thesis under the supervision of Prof. Gianni Cardini.
- **September 2009** Master Degree in Chemistry (summa cum laude) at the University of Florence (Italy) with a thesis entitled '*Spectral Analysis with Wavelet Transform in Molecular Dynamics*' under the supervision of Prof. Vincenzo Schettino.
- **March 2013** International Ph.D. in Atomic and Molecular Spectroscopy at the European Laboratory for NonLinear Spectroscopy (LENS –University of Florence, Italy) with a thesis entitled '*Modelling of spectroscopic and structural properties using molecular dynamics*' under the supervision of Prof.s Vincenzo Schettino and Roberto Righini

VISITS AND STAYS

- **June 2016** Visiting scientist at *École Nationale Supérieure de Chimie de Paris* (ENSCP) - *Chemie Paristech*, Paris (France)

PREVIOUS POSITIONS AND FELLOSHIPS

- **From April 2013 to March 2016.** Postdoctoral position at UNIMORE (Italy).
- **From April 2016 to April 2017.** Postdoctoral position at UNIMORE (Italy).
- **From May 2017 to December 2018.** Postdoctoral position at Universiteit Gent (UGent) in Belgium.
- **From February 2019 to July 2020.** Researcher in Physical Chemistry at CNRS (*Centre National de la Recherche Scientifique*) – Paris (France)
- **From September 2020 to October 2021.** Researcher (RTDa) at POLITO (*Polytechnic University of Turin* – Italy).

MEMBERSHIPS AND APPOINTMENTS

- Member of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society (SCI).
- Member of the Division of Physical Chemistry of the Italian Chemical Society (SCI).
- Member of the panel of the Ph.D. course "Models and Methods for Materials and Environmental Sciences" of UNIMORE - DSGC department (from the academic year 2022/2023).

ORGANIZATION OF SCIENTIFIC MEETINGS AND SCHOOLS

- Member of the Organizing Committee of the European Congress of Molecular Spectroscopy EUCMOS XXX, Florence, Italy.
- Member of the Organizing Committee of the VII Congress of Division of Theoretical and Computational Chemistry (SCI), 2022, Modena, Italy.
- Guest Editor of the *Nanomaterials* (IF 5.719) – MDPI.

FUNDING AND PROJECTS

As PI or deputy-PI:

- Project PRIN (Project of relevant national interest) called Enzylearning. Call PRIN 2022.

As participant:

- Project ERC Consolidator (European Research Council) "Modeling approaches toward bioinspired materials" of the professor Giovanni Maria Pavan (POLITO, Turin).
- Project ERC Consolidator (European Research Council) "Escaping from the Franck-Condon region: a theoretical approach to describe molecular structural reorganization for reversible energy and information storage at the excited state" of the professor Ilaria Ciofini (CNRS, Paris).
- Project ERC Consolidator (European Research Council) "First Principle Chemical Kinetics in Nanoporous Materials" of the professor Veronique Van Spreybroeck (UGent, Belgium).
- Project UniMORE (Università di Modena e Reggio Emilia) "Computational study of physico-chemical properties of metallic nanoparticles functionalized with organic molecules" of the professor Alfonso Pedone.
- Project FIRB (Futuro in Ricerca) "Novel Multiscale Theoretical/Computational Strategies for the Design of Photo and Thermo responsive Hybrid Organic Inorganic Components for Nanoelectronic Circuits" of the professor Alfonso Pedone (UNIMORE).

ACTIVITIES IN REFERRED SCIENTIFIC JOURNALS.

Reviewer for these scientific Journals:

- *The Journal of Physical Chemistry*, *ACS Nano, Accounts of Chemical Research* (American Chemical Society)
- *Physical Chemistry Chemical Physics*, *Chemical Communications* (Royal Society of Chemistry)
- *Theoretical Chemistry Accounts* (Springer**)**
- *Chemical Engineering Journal, Journal of Materials Research and Technology, Vibrational Spectroscopy, Computational and Theoretical Chemistry*, *Journal of Molecular Structure, Thin Solid Films, Journal of Molecular Graphics and Modelling* (Elsevier)
- *Journal of Raman Spectroscopy, Chem Phys Chem* (Wiley**)**
- *International Journal of Modern Physics B* (World Scientific**)**
- *Materials, Nanomaterials, Metals, Applied Sciences*, *Inorganics, Molecules, Coatings, Sensors* (MDPI**)**

SELECTED INVITED PRESENTATIONS

- **F. Muniz-Miranda**, "*Studies on the optoelectronic properties of metal nanoclusters and complexes*", Congress of the Division of Theoretical and Computational Chemistry (2018),Trieste (Italy), September 2018.

- **F. Muniz-Miranda** "*Computational investigation of vibrational and UV-vis spectra in molecular and metal systems*", Center for Molecular Modeling (CMM), Gent University (Belgium), December 2016.
- **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Optical Features of Au and Ag-based Nanocluster*, Conference on "Charge Transfer Modeling in Chemistry: new methods and solutions for a longstanding problem", Paris (France), April 2015.

AWARDS

- **2018**: Prize "Eolo Scrocco" of the Italian Chemical Society (SCI).
  http://www.unifimagazine.it/riconoscimento-giovane-studioso-fiorentino/
  https://www.soc.chim.it/sites/default/files/Comunicato_Premi_2018.pdf

- **2014**: Prize "Migliore tesi di Dottorato" – University of Florence (Italy), along with the publication of the doctoral dissertetion by the publishing company FUP (Firenze University Press)
  https://www.fupress.com/autori/muniz-miranda-francesco/134220

SUPERVISION OF PhD STUDENTS AND POSTDOCTORAL FELLOWS

- 2016: co-tutor for the thesis in Chemistry by Ms. Federica Lodesani, UNIMORE.
- 2017-2018: supervisor of the doctoral students Mr. Kim Phan and Ms. Liesbeth De Brucker (Ghent University – Belgium).
- 2017-2018: supervisor of the Master thesis of Ms. Léon Huet (Chimie ParisTech, Paris).

TEACHING ACTIVITIES

- 2014/2015, 2015/2016, 2016/2017: Teaching assistance with seminars and lectures in the calculus laboratory for the course "*Physical Chemistry and Molecular Spectroscopy*" of the master's degree in Chemistry, UniMORE for a total of about 30 lectures.
- • 2015/2016: Assistance in laboratory exercises for the "*Physical Chemistry I*" course of the three-year degree in Chemistry, UniMORE for a total of about 10 hours.
- 2017/2018: Teaching assistance for the "*Molecular Structure*" course (in English), for students of the Master in Physics and Engineering of the University of Ghent (Belgium), with additional lessons and use of software, for a total about 10 hours frontal.
- 2019, 2020: Teaching of the "*Chemical Bonding*" course (16 hours of lectures, of which 12 hours in 2019 and 4 hours in 2020, in English), for third year students of the Bachelor of Science in Chemical Engineering , at École Nationale Supérieure de Chimie de Paris, as Researcher in Physical Chemistry.
- 2019: Teaching of the "*Molecular Modeling*" course (8 hours of lectures, in English), for third year students of the degree course in Chemical Engineering, at École Nationale Supérieure de Chimie de Paris, as Researcher in Physical Chemistry.
- 2021-2022 - onwards: Teaching of the "*Physical Chemistry – Molecular Spectroscopy*" course at the University of Modena and Reggio Emilia (Italy) of the master degree in Chemistry.
- 2023-2024 - onwards: Teaching of the "*Chemico-Physical Methods for Materials Characterization*" course at the University of Modena and Reggio Emilia (Italy) of the bachelor degree in Chemistry.

MAJOR COLLABORATIONS

Prof. Maria Cristina Menziani, Università di Modena e Reggio Emilia
Email: mariacristina.menziani@unimore.it

Prof. Alfonso Pedone, Università di Modena e Reggio Emilia,
Email: alfonso.pedone@unimore.it

Prof. Veronique Van Speybroeck, University of Ghent (Belgium)
Email: veronique.vanspeybroeck@ugent.be

Prof. Carlo Adamo, École nationale supérieure de chimie de Paris
Email: carlo-adamo@chimie-paristech.fr

BRIEF DESCRIPTION OF THE RESEARCH ACTIVITY

I perform calculations in computational chemistry to recover/interpret/predict: reaction barriers, dynamical behaviour of molecules, UV-Vis and vibrational spectra, charge-transfer.

OTHER INFORMATION

BIBLIOMETRIC INDICATORS AND SCIENTIFIC PRODUCTION

Total number of publications in scientific journals: 48 (Scopus), 56 (Google Scholar)
Total number of book chapters: 2
Total number of other publications: 1 book
Total number of citations: 850 (Scopus), 986 (Google Scholar)
h-index: 18 (Scopus), 20 (Google Scholar)
Average number of citations per publication: 15.5 (Scopus)
Average number of citations per year: 2011 (5), 2012 (16), 2013 (7), 2014 (28), 2015 (48), 2016 (75), 2017 (55), 2018 (69), 2019 (88), 2020 (106), 2021 (134), 2022 (123), 2023 (98) – Scopus – average per year 65.34

PUBLIC ENGAGEMENT

"Notte della ricerca" September 2022 - Modena
"Scuola di chimica di base", September 2022, Modena
"Scuola di chimica di base", February 2023, Modena

LIST OF SCIENTIFIC PUBLICATIONS ON INTERNATIONAL JOURNALS WITH IF.

1) M. Muniz-Miranda, **F. Muniz-Miranda**, M.C. Menziani, A. Pedone, *Can DFT Calculations Provide Useful Information for SERS Applications?*, Molecules, **2023**, 28, 575, Doi: 10.3390/molecules28020573
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 4.600

2) **F. Muniz-Miranda**, A. Pedone, M.C. Menziani, M. Muniz-Miranda, *DFT and TD-DFT Study of the Chemical Effect in the SERS Spectra of Piperidine Adsorbed on Silver Colloidal Nanoparticles*, Nanomaterials, **2022**, 12, 2907, Doi: 10.3390/nano12172907
Luogo di pubblicazione: Basilea (Svizzera).

Editore: MDPI
Impact Factor: 5.719

3) R. Capelli, **F. Muniz-Miranda**, G.M. Pavan, *Ephemeral ice-like local environments in classical rigid models of liquid water*, The Journal of Chemical Physics, **2022**, 156, 214503, Doi: 10.1063/5.0088599
Luogo di pubblicazione: College Park (Maryland, USA)
Editore: American Institute of Physics
Impact Factor: 3.488

4) M. Filez, C. Caratelli, M. Rivera-Torrente, **F. Muniz-**M**iranda**, M. Hoek, M. Altelaar, A. J.R. Heck, V. Van Speybroeck, B.M. Weckhuysen, *Elucidation of the pre-nucleation phase directing metal-organic framework formation*, Cell Reports Physical Science, **2021**, 2, 100680, Doi: 10.1016/j.xcrp.2021.100680
Luogo di pubblicazione:
Editore: Elsevier
Impact Factor: 7.832

5) **F. Muniz-Miranda**, *Computational Approaches to the Electronic Properties of Noble Metal Nanoclusters Protected by Organic Ligands*, Nanomaterials, 2021, 11, 2409 (pp. 1-12), Doi: 10.3390/nano11092409
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 5.719

6) C. Micheletti, P. Minei, M. Carlotti, V. Mattoli, **F. Muniz-Miranda,** A. Perfetto, I. Ciofini, C. Adamo, G. Ruggeri, A. Pucci, *Mechanochromic LLDPE Films doped with NIR Reflective Paliogen Black,* Macromolecular Rapid Communications, **2021**, 42, 2000426 (pp. 1-8), Doi: 10.1002/marc.202000426
Luogo di pubblicazione: Weinheim (Germania).
Editore: John Wiley & Sons
Impact Factor: 5.734

7) L. Huet, A. Perfetto, **F. Muniz-Miranda** (corresponding), M. Campetella, C. Adamo, I. Ciofini, *General density-based index to analyze charge transfer phenomena: from models to butterfly molecules,* Journal of Chemical Theory and Computation, **2020**, 16, 4543–4553, Doi: 10.1021/acs.jctc.0c00296
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 6.006

8) S. M. J. Rogge, P. G. Yot, J. Jacobsen, **F. Muniz-Miranda**, S. Vandenbrande, J. Gosch, V. Ortiz, I. E. Collings, S. Devautour-Vinot, G. Maurin, N. Stock, V. Van Speybroeck, *Charting the Metal-Dependent High-Pressure Stability of Bimetallic UiO-66 Materials*, ACS Materials Letters, **2020**, *2*, 438-445, Doi: 10.1021/acsmaterialslett.0c00042
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 8.312

9) S. Abednatanzi, P. G, Derakhshandeh, P. Tack, **F. Muniz-Miranda**, Y.Y. Liu, J. Everaert, M. Meledina, F. Vanden Bussche, L. Vincze, C. V. Stevens, V. Van Speybroeck, H. Vrielinck, F.

Callens, K. Leus, P. Van Der Voort, *Elucidating the Promotional Effect of a Covalent Triazine Framework in Aerobic Oxidation,* Applied Catalysis B: Environmental, **2020**, *269*, 118769, Doi: 10.1016/j.apcatb.2020.118769
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier
Impact Factor: 19.503

10) M. Muniz-Miranda, A. Zoppi, **F. Muniz-Miranda**, N. Calisi, *Palladium Oxide Nanoparticles: Preparation, Characterization and Catalytic Activity Evaluation,* Coatings **2020**, *10*, 207 (pp. 1-10), Doi: 10.3390/coatings10030207
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 2.881

11) M. Muniz-Miranda, **F. Muniz-Miranda**, E. Giorgetti, *Spectroscopic and Microscopic Analyses of Fe_3O_4/Au Nanoparticles Obtained by Laser Ablation in Water*, Nanomaterials, **2020**, *10*, 132 (pp. 1-14), Doi: 10.3390/nano10010132
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 5.076

12) **F. Muniz-Miranda,** P. Minei, L. Contiero, F. Labat, I. Ciofini, C. Adamo, F. Bellina, A. Pucci, *Aggregation effects on pigment coatings: Pigment Red 179 as case study*, ACS Omega, **2019**, *4,* 20315-20323, Doi: 10.1021/acsomega.9b02819
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 3.512

13) A. Zoppi, S. Caporali, **F. Muniz-Miranda**, A. Pedone, M. Muniz-Miranda, *Adsorption of Trans-Zeatin on Laser-Ablated Gold Nanoparticles for Transport into Plant Cells and Growth Stimulation*, ACS Applied Nano Materials **2019**, *2*, 7319−7327, Doi: 10.1021/acsanm.9b01801
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 5.097

14) I. Lopez-Tocon, S. Valdivia, J. Soto, J. C. Otero, **F. Muniz-Miranda**, M. C. Menziani, M. Muniz-Miranda, *A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles,* Nanomaterials, **2019**, *9*, 1211; Doi: 10.3390/nano9091211
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 5.076

15) **F. Muniz-Miranda**, L. De Bruecker, A. De Vos, F. Vanden Bussche, C. V. Stevens, P. Van Der Voort, K. Lejaeghere, V. Van Speybroeck, *Optical Properties of Isolated and Covalent Organic Framework-Embedded Ruthenium Complexes*, Journal of Physical Chemistry A, **2019**, *123*, 6854−6867, Doi: 10.1021/acs.jpca.9b05216
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 2.781

16) S. Caporali, **F. Muniz-Miranda**, A. Pedone, M. Muniz-Miranda, *SERS, XPS and DFT Study of Xanthine Adsorbed on Citrate-Stabilized Gold Nanoparticles,* Sensors, **2019**, *19*, 2700 (pp. 1-10), Doi: 10.3390/s19122700
Luogo di pubblicazione: Basilea (Svizzera).
Editore: MDPI
Impact Factor: 3.576

17) A. De Vos, K. Lejaeghere, **F. Muniz Miranda**, C. V. Stevens, P. Van Der Voort, V. Van Speybroeck, *Electronic properties of heterogenized Ru(II) polypyridyl photoredox complexes on covalent triazine frameworks,* Journal of Materials Chemistry A, **2019**, *7*, 8433-8442, Doi: 10.1039/C9TA00573K
Luogo di pubblicazione: Londra (UK).
Editore. Royal Society of Chemistry
Impact Factor: 12.732

18) N. Tahir, **F. Muniz-Miranda**, J. Everaert, P. Tack, T. Heugebaert, K. Leus, L. Vincze, C. V. Stevens, V. Van Speybroeck, P. Van Der Voort, *Immobilization of Ir(I) complex on covalent triazine frameworks for C-H borylation reactions: A combined experimental and computational study*, Journal of Catalysis, 2019, *371*, 135-143, Doi: 10.1016/j.jcat.2019.01.030
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier
Impact Factor: 7.920

19) M. Muniz-Miranda, **F. Muniz-Miranda**, S. Caporali, N. Calisi, A. Pedone, *SERS, XPS and DFT investigation on palladium surfaces coated with 2,2'-bipyridine monolayers*, Applied Surface Science, **2018**, *457*, 98-103, Doi: 10.1016/j.apsusc.2018.06.232
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier
Impact Factor: 6.707

20) **F. Muniz-Miranda**, A. Pedone, M. Muniz-Miranda, *Raman and computational study on the adsorption of xanthine on silver nanocolloids*, ACS Omega, **2018**, *3,* 13530-13537, Doi: 10.1021/acsomega.8b02174
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 3.512

21) C. Gellini, **F. Muniz-Miranda**, A. Pedone, M. Muniz-Miranda, *SERS active Ag–SiO2 nanoparticles obtained by laser ablation of silver in colloidal silica*, Beilstein Journal of Nanotechnology, **2018**, *9,* 2396-2404, Doi: 10.3762/bjnano.9.224
Luogo di pubblicazione: Francoforte (Germania).
Editore: Beilstein Institute
Impact Factor: 3.649

22) M. Muniz-Miranda, **F. Muniz-Miranda**, A. Pedone , *SERS and DFT investigation on push-pull molecules: 4-Dimethylamino- 4'-nitrostilbene adsorbed on silver colloidal nanoparticles*, ChemistrySelect, 2018, *3*, 8698-8702, Doi: 10.1002/slct.201801825
Luogo di pubblicazione: Chichester (UK).
Editore: Wiley-VCH
Impact Factor: 2.109

23) F. Tavanti, **F. Muniz-Miranda**, A. Pedone, *The effect of alkaline cation on the intercalation of Carbon Dioxide in Sepiolite Minerals: a Molecular Dynamics Investigation,* Frontiers in Materials, **2018**, *5*, article 12, pp. 1-9, Doi: 10.3389/fmats.2018.00012
Luogo di pubblicazione: Losanna (Svizzera).
Editore: Frontiers Media
Impact Factor: 3.515

24) **F. Muniz-Miranda**, A. Pedone, M. Muniz-Miranda, *Spectroscopic and DFT investigation on the photo-chemical properties of a push-pull chromophore: 4-Dimethylamino-4'-nitrostilbene*, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **2018**, *190*, 33-39, Doi: 10.1016/j.saa.2017.08.072
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier
Impact Factor: 4.098

25) C. Gellini, F. L. Deepak, M. Muniz-Miranda, S. Caporali**, F. Muniz-Miranda**, A. Pedone, C. Innocenti, C. Sangregorio, *Magneto-Plasmonic Colloidal Nanoparticles Obtained by Laser Ablation of Nickel and Silver Targets in Water,* Journal of Physical Chemistry C, **2017**, *121*, 3597-3606, Doi: 10.1021/acs.jpcc.6b11628
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 4.126

26) **F. Muniz-Miranda**, F. Lodesani, F. Tavanti, D.Presti, D. Malferrari, A. Pedone, *Supercritical CO2 confined in Palygorskite and Sepiolite Minerals. A classical Molecular Dynamics investigation*, Journal of Physical Chemistry C, **2016**, *120*, 26945-26954, Doi: 10.1021/acs.jpcc.6b09983
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 4.126

27) A. Pedone, **F. Muniz-Miranda**, A. Tilocca, M. C. Menziani, *The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations,* Biomedical glasses, **2016**, 2, pp. 19-28, Doi: 10.1515/bglass-2016-0003
Luogo di pubblicazione: Varsavia (Polonia).
Editore: De Gruyter
Impact Factor: 2.286

28) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Assessment of the basis set effect on the structural and electronic properties of organic-protected gold nanoclusters*, Theoretical Chemistry Accounts, **2016**, 135:94, pp. 1-9, Doi: 10.1007/s00214-016-1856-2
Luogo di pubblicazione: Berlino (Germania).
Editore: Springer
Impact Factor: 1.702

29) M. Muniz-Miranda, **F. Muniz-Miranda**, A. Pedone, *Raman and DFT study of methimazole chemisorbed on gold colloidal nanoparticles*, Physical Chemistry Chemical Physics, **2016**, 18, 5974-5980, Doi: 10.1039/C5CP07597A
Luogo di pubblicazione: Londra (UK).
Editore. Royal Society of Chemistry
Impact Factor: 3.676

30) **F. Muniz-Miranda**, D. Presti, M. C. Menziani, A. Pedone, *Electronic and optical properties of the Au_{22}[1,8-bis(diphenylphosphino) octane]$_6$ nanoclusters disclosed by DFT and TD-DFT calculations*, Theoretical Chemistry Accounts, **2016**, 135:5, p.1-9, Doi: 10.1007/s00214-015-1764-x
Luogo di pubblicazione: Berlino (Germania).
Editore: Springer
Impact Factor: 1.702

31) **F. Muniz-Miranda**, A. Pedone, G. Battistelli, M. Montalti, J. Bloino, V. Barone, *Benchmarking TD-DFT against Vibrationally Resolved Absorption Spectra at Room Temperature: 7-Aminocoumarins as Test Cases*, Journal of Chemical Theory and Computation, **2015**, 11, 5371−5384, Doi: 10.1021/acs.jctc.5b00750
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 6.006

32) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *DFT and TD-DFT Assessment of the Structural and Optoelectronic Properties of Organic-Ag_{14} Nanocluster*, Journal of Physical Chemistry A, **2015**, 119, 5088–5098, Doi:10.1021/jp507679f
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 2.781

33) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Influence of Silver Doping on the Photoluminescence of Protected Ag_nAu_{25-n} Nanoclusters: A Time-Dependent Density Functional Theory Investigation,* Journal of Physical Chemistry C, **2015**, 119, 10766-10775, Doi: 10.1021/acs.jpcc.5b02655
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 4.126

34) M. Muniz-Miranda, **F. Muniz-Miranda**, S. Caporali*, SERS and DFT study of copper surfaces coated with corrosion inhibitor*, Beilstein Journal of Nanotechnology, **2014**, 5, 2489-2497, Doi: 10.3762/bjnano.5.258
Luogo di pubblicazione: Francoforte (Germania)
Editore: Beilstein Institute
Impact Factor: 3.649

35) M. Muniz-Miranda, B. Pergolese, **F. Muniz-Miranda**, S. Caporali, *SERS effect from Pd surfaces coated with thin films of Ag colloidal nanoparticles*, Journal of Alloys and Compounds, **2014**, 615, S357-S360, Doi: 10.1016/j.jallcom.2013.12.063
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier
Impact Factor: 5.315

36) A. J. Clark, A. Cornia, F. Felluga, A. Gennaro, F. Ghelfi, A. A. Isse, M. C. Menziani, **F. Muniz-Miranda**, F. Roncaglia, D. Spinelli, *Arylsulfonyl Groups: the Best Cyclization Auxiliaries for the Preparation of ATRC γ-Lactams can be Acidolytically Removed*, European Journal of Organic Chemistry, **2014**, 30, 6734-6745, Doi: 10.1002/ejoc.201402769
Luogo di pubblicazione: Chichester (UK).

Editore: Wiley-VCH
Impact Factor: 3.021

37) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters*, Physical Chemistry Chemical Physics, **2014**, 16, 18749-18758, Doi: 10.1039/c4cp02506g
Luogo di pubblicazione: Londra (UK).
Editore. Royal Society of Chemistry
Impact Factor: 3.676

38) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Assessment of Exchange-Correlation Functionals in Reproducing the Structure and Optical Gap of Organic-Protected Gold Nanoclusters*, Journal of Physical Chemistry C, **2014**, 118, 7532-7544, Doi: 10.1021/jp411483x
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 4.126

39) **F. Muniz-Miranda**, M. Pagliai, G. Cardini, R. Righini, *Hydrogen-bond Effects in the Vibrational Spectra of 1,3-Propanediol in Acetonitrile: Ab initio and Experimental Study*, Journal of Chemical Physics, **2012**, 137, 244501, Doi: 10.1063/1.4770499
Luogo di pubblicazione: College Park (Maryland, USA)
Editore: American Institute of Physics
Impact Factor: 3.488

40) M. Pagliai, **F. Muniz-Miranda**, V. Schettino, M. Muniz-Miranda, *Competitive Solvation and Chemisorption in Silver Colloidal Suspensions*, Progress in Colloid and Polymer Science (Supplement of Colloid & Polymer Science), **2012**, 139, 39-44, Doi: 10.1007/978-3-642-28974-3_8
Luogo di pubblicazione: Berlino (Germania)
Editore: Springer
Impact Factor: 1.931

41) **F. Muniz-Miranda**, M. Pagliai, G. Cardini, R. Righini, *Bifurcated Hydrogen Bond in Lithium Nitrate Trihydrate Probed by ab Initio Molecular Dynamics*, Journal of Physical Chemistry A, **2012**, 116, 2147-2153, Doi: 10.1021/jp2120115
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 2.781

42) V. Volkov, R. Chelli, **F. Muniz-Miranda**, R. Righini, *Structural Properties of a Membrane Associated Anchor Dipeptide*, Journal of Physical Chemistry B, **2011**, 115, 5294-5303, Doi: 10.1021/jp109284z
Luogo di pubblicazione: Washington (USA).
Editore: American Chemical Society
Impact Factor: 2.991

43) M. Pagliai, **F. Muniz-Miranda**, G. Cardini, R. Righini, V. Schettino*, Spectroscopic properties with a combined approach of ab initio molecular dynamics and wavelet analysis,* Journal of Molecular Structure, **2011**, 993, 438-442, Doi: 10.1016/j.molstruc.2011.02.007
Luogo di pubblicazione: Amsterdam (Paesi Bassi).
Editore: Elsevier

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44) **F. Muniz-Miranda**, M. Pagliai, G. Cardini, V. Schettino, *Wavelet Transform for Spectroscopic Analysis: Application to Diols in Water*, Journal of Chemical Theory and Computation, **2011**, 7, 1109-1118, Doi: 10.1021/ct100625e
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