Résumé of Francesco MUNIZ-MIRANDA

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Born:	**/**/1983, Fiesole (Metropolitan City of Florence), Italy
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Languages:	*Italian* (mother tongue), *English* (C2 written, C1 oral)

RESEARCH JOBS

November 2021 → now: Tenure-Track Assistant Professor (RTD/B) of Physical Chemistry
at the University of Modena and Reggio Emilia University (UniMORE), Department of Chemical and Geological Sciences (DSCG), Italy.
Homepage: https://personale.unimore.it/rubrica/dettaglio/fmunizmi

September 2020 → October 2021: Research Assistant Professor (RTD/A) of Physical Chemistry
at the Politecnico di Torino (PoliTO), Department of Applied Science and Technology (DiSAT) in the group lead by Prof. Dr. Giovanni Maria Pavan.

January 2019 → July 2020: *Chercheur en Chimie Physique*
at CNRS (Centre national de la recherche scientifique), attached to the *École nationale supérieure de chimie de Paris* (Chimie ParisTech) on the ERC project "Striges" of Dr. Ciofini (Director of Research, CNRS). I worked on the use of charge transfer descriptors in UV-Vis excitations and modeling of pressure-induced photochromism.

May 2017 → December 2018: Post-doctoral fellow
at Universiteit Gent (UGent), Belgium, at the Centrum voor Moleculaire modellering (within Prof. Van Speybroeck's project "Advanced electronic structure characterization of COF materials and metal complexes towards effective photoredox catalysts")

April 2016 → April 2017: Post-doctoral scholar
at the University of Modena and Reggio Emilia University (UniMORE), Department of Chemical and Geological Sciences (DSCG), Italy, on classical simulations of CO_2 adsorption in clay minerals under the supervision of Prof. Dr. Alfonso Pedone.

April 2013 → April 2016: Post-doctoral scholar
at the University of Modena and Reggio Emilia University (UniMORE), Department of Chemical and Geological Sciences (DSCG), Italy. I worked on TD-DFT simulations of the opto-electronic properties of gold or silver nanoclusters, under the supervision of Dr. Alfonso Pedone (FIRB funding).

January 2010 → March 2013 : Ph.D. student
at the European Laboratory for Non-Linear Spectroscopy (LENS), University of Florence (UniFI), Sesto Fiorentino, Italy, under the supervision of Prof. Em. Vincenzo Schettino.
As a computational chemist embedded in a molecular spectroscopy laboratory, I performed Car-Parrinello molecular dynamics simulations of hydrogen-bonded systems to recover their vibrational spectra with a wavelet-transform code that I wrote. Wavelet-transform resolves a

signal in both time and frequency domains, thus allowing to correlate structural and spectroscopic properties.
My Ph.D. dissertation was awarded publication by the Firenze University Press (FUP) within the "Prize for Ph.D. thesis" initiative ("*Premio tesi di Dottorato*"). It can be downloaded at the following link:
http://www.fupress.com/catalogo/modelling-of-spectroscopic-and-structural-properties-using-molecular-dynamics/2880

EDUCATION

- International Ph.D. Degree ("*Dottorato Internazionale di Ricerca*") in **Atomic and Molecular Spectroscopy**, March 15, 2013, LENS (European Laboratory for Non-Linear Spectroscopy).
  Advisors: Prof. Em. Vincenzo Schettino & Prof. Dr. Roberto Righini (University of Florence and LENS)
  International referees: Prof. Dr. Claus Jørgen Nielsen (Univ. of Oslo)
  Prof. Federico Moran (Univ. of Madrid)
  Prof. Ana Isabel Cremades Rodriguez (Univ. of Madrid)

- Master Degree ("*Laurea Specialistica*") in **Chemistry**, September 2009, University of Florence.
  Advisor: Prof. Em. Vincenzo Schettino
  full marks and honors (110/110 "c*um laude*")

- Bachelor Degree ("*Laurea Triennale*") in **Chemistry**, April 2007, University of Florence.
  Advisor: Prof. Dr. Gianni Cardini
  full marks (110/110)

AWARDS AND PRIZES

- **2018**: "Eolo Scrocco" prize of the Theoretical and Computational Chemistry Division (DCTC) of the Italian Chemical Society (SCI) for the best research work in the field performed in Italy by a researcher under 35 years of age.

- **2014**: "Best Ph.D. Prize" for the scientific doctoral dissertation at the University of Florence.

QUALIFICATIONS

- **2021** I got the Italian "National Scientific Habilitation" (ASN, "*Abilitazione Scientifica Nazionale*") for the position of Full Professor in the field "Theoretical Physics (of Condensed Matter)" (Italian codename 02/B2).

- **2019** I got the Italian "National Scientific Habilitation" (ASN, "*Abilitazione Scientifica Nazionale*") for the position of Associate Professor in the field "Theoretical Physics (of Condensed Matter)" (Italian codename 02/B2).

- **2019** I got the Italian "National Scientific Habilitation" (ASN, "*Abilitazione Scientifica Nazionale*") for the position of Associate Professor in the field "Methods and Models in Chemistry" (Italian codename 03/A2), which includes Physical Chemistry.

- **2018** I got the Italian "National Scientific Habilitation" (ASN, "*Abilitazione Scientifica Nazionale*") for the position of Associate Professor in the field "General and Inorganic Chemistry" (Italian codename 03/B1).

- **2009** I got the Italian state qualification to work as a "senior" chemist (M.Sc. level).

VISITING SCIENTIST

Visiting scientist at *École Nationale Supérieure de Chimie de Paris* (ENSCP) - *Chimie Paristech*, Paris (France), Prof. Carlo Adamo's group, 1 month (1 − 30 June, 2016).

ACTIVITIES AS REVIEWER IN SCIENTIFIC JOURNALS and ACADEMY

Since 2015, I have been assigned review duty by:
The Journal of Physical Chemistry (6 times), *ACS Nano, and Accounts of Chemical Research* for ACS; *Physical Chemistry Chemical Physics* (3 times) and *Chemical Communications* (4 times) for RSC; *Theoretical Chemistry Accounts* for Springer (5 times);
Vibrational Spectroscopy (2 times), *Chemical Engineering Journal* (2 times), *Computational and Theoretical Chemistry*, *Journal of Molecular Structure*, *Journal of Molecular Graphics and Modelling* and *Materials Science in Semiconductor Processing* for Elsevier;
ChemPhysChem and *Journal of Raman Spectroscopy* (2 times) for Wiley;
International Journal of Modern Physics B (2 times) for World Scientific;
Materials, *Nanomaterials* (6 times), *Metals*, *Applied Sciences*, *Inorganics*, *Molecules*, *Coatings*, and *Sensors* for MDPI.

In April, 2021, I have been invited to be reviewer for the Italian ANVUR, the state organization that assess the research of universities (VQR, *Valutazione della Qualità della Ricerca*, "Evaluation of the Quality of Research") for the fields of Physical Chemistry, Inorganic Chemistry and Physics of Condensed Matter.

EDITORIAL ACTIVITY

- I have been invited multiple times to act as guest editor for special issues of the MDPI journal *Nanomaterials*. I accepted in September 2021.
- I have been invited to act as guest editor for a special issue on Advances in Metal Nanoparticles of the MDPI journal *Materials* in February, 2020.
- I have been invited to join the editorial board of the MDPI journal *Computation* in July, 2019.

MEMBERSHIPS

- Member of the American Chemical Society (ACS) in 2018-2019, card n° 31771560.
- Member of the Division of Theoretical and Computational Chemistry (DTCC) of the Italian Chemical Society (SCI) since 2013, of the Physical Chemistry division since 2020, and of the division of Chemistry for Technology since 2021. Card n° 19074.

Participation to SCHOOLS AND WORKSHOPS

- *"MSSC2018 – Ab initio Modelling in Solid State Chemistry"*, Turin (Italy), 2018.
- *"Excited States in Complex Systems*", Paris (France), 2016.
- *"Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA"*, CECAM Workshop, Mainz (Germany), 2016.
- *"Calculation of Solid-State NMR and EPR Parametres Using the GIPAW Method"*, CECAM Tutorial, ETH, Zurig (Swizerland), 2013.
- "*European Summer School of Scientific Visualization*", CINECA, Bologna (Italy), 2012.
- "*Introduction to Fortran 90*", CINECA, Bologna (Italy), 2011
- *"HPC UserDay 2011"*, CINECA, Bologna (Italy), 2011

- *"C for scientific programming"*, CINECA, Bologna (Italy), 2010.
- *VI "Advanced School of Parallel Programming"*, CINECA, Bologna (Italy), 2010.
- "*Computational spectroscopy using Quantum Espresso and related codes*", CECAM Tutorial, SISSA, Trieste (Italy), 2010.
- *XIX "Summer School of Parallel Programming"*, CINECA, Bologna (Italy), 2010.
- *"Frontiers in Atomic Physics"*, Florence (Italy), 2010.

TEACHING ACTIVITY

- *2019, 2020*: **Teacher** for the course "*Liaison Chimique*" (Chemical Bonding, taught in English) at the École nationale supérieure de chimie de Paris (3rd year course). Syllabus: Hydrogen atom, Spin operators, Hydrogen Molecule, Hartree product, Slater determinant, Hartree-Fock calculations on HF and Li_2.
- *2017/2018:* **Teaching Assistant** for the course "*Molecular Structure*" (in English), University of Ghent (Belgium)
- *2017/2018:* **Laboratory Assistant**. Practical exercises with Gaussian 16 software for Master students in Physics and Engineering, University of Ghent (Belgium).
- *2015/2016*: **Laboratory Assistant**. Course "*Physical Chemistry I*", Degree in Chemistry, University of Modena and Reggio Emilia, Italy
- *2014/2015, 2015/2016, 2016/2017:* **Teaching Assistant**. Lessons and computational exercises for the Course "*Physical Chemistry and Molecular Spectroscopy*", University of Modena and Reggio Emilia, Italy

INVITED TALKS

1) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, "*Optical Features of Au and Ag-based Nanoclusters"*, CECAM Conference "Charge Transfer Modelling in Chemistry: new methods and solutions for a long-standing problem", Paris (France), April 2015.

2) **F. Muniz-Miranda** "*Computational investigation of vibrational and UV-vis spectra in molecular and metal systems*", Center for Molecular Modeling (CMM), Ghent University (Belgium), December 2016.

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

COMMUNICATIONS TO NATIONAL AND INTERNATIONAL CONFERENCES

1) **F. Muniz-Miranda***, F. Labat, C. Adamo, I. Ciofini, *Modeling aggregation effects on UV-Vis spectra of dyes: Pigment Red 179 as case study*, 18th International Conference on Density Functional Theory and its Applications, Alicante (Spain), July 2019.

2) A. De Vos, K. Lejaeghere, **F. Muniz-Miranda**, P. Van der Voort,V. Van Speybroeck, *Insight in heterogeneous photocatalysis by anchoring a photoactive Ru-complex on a Covalent Triazine Framework*, MOFSIM 2019, Ghent (Belgium), April 2019.

3) A. De Vos, K. Lejaeghere, **F. Muniz-Miranda**, P. Van der Voort, V. Van Speybroeck, *First-principles insight into Heterogeneous Photocatalysis at photoactive Ru-complexes on Covalent Triazine Frameworks,*

6th International Conference on Metal-Organic Frameworks, Auckland (New Zealand), December 2018.

4) A. De Vos, **F. Muniz-Miranda**, P. Van der Voort, V. Van Speybroeck, K. Lejaeghere, *Insight in heterogeneous photo catalysis by anchoring a photo active Ru-complex on a Covalent Triazine Framework*, "Computational Spectroscopy: bridging theory and experiment" Meeting, Como (Italy), September 2018.

5) **F. Muniz-Miranda***, *Computational UV-vis spectroscopy*, Symposium "Modeling of nanoporous materials at the nanoscale", Utrecht University, Utrecht (Netherlands), September 2018.

6) S. Caporali, **F. Muniz-Miranda**, M. Muniz-Miranda, *Adsorption of xanthine on citrate-stabilized gold nanoparticles*, 25th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2018), Rome (Italy), July 2018.

7) **F. Muniz-Miranda***, M. C. Menziani, A. Pedone, *Optical Excitations in Au and Ag nanoclusters*, Excited States in Complex Systems, ESCS 2016, ChimieParisTech, Paris (France), November 2016.

8) **F. Muniz-Miranda***, F. Lodesani, F. Tavanti, D. Presti, D. Malferrari, A. Pedone, *Supercritical CO_2 Confined in Palygorskite and Sepiolite Minerals: A Classical Molecular Dynamics Investigation,* DCTC-SCI Congress, Pisa (Italy), October 2016.

9) **F. Muniz-Miranda**, F. Tavanti, M. C. Menziani, A. Pedone, *Molecular Modelling of metal nanoclusters and nanoparticles: from TDDFT calculations to coarse grained MD simulations*, Workshop "Nanostructured Metal Optics", Scuola Normale Superiore, Pisa (Italy), April 2016.

10) M. C. Menziani, **F. Muniz-Miranda**, A. Pedone, *Modeling unconventional bioactive glasses*, 2nd International Workshop on "Challenges of Atomistic Simulations of Glasses and Amorphous Materials", Wuhan (China), June 2015.

11) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Structural and Optical Properties of organically Protected Gold and Silver Nanoclusters*, Winter Modelling 2014 - Special Edition, Pisa (Italy), December 2014.

12) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Structural and optical properties of gold and silver nanoclusters*, WATOC Conference, Santiago (Chile), October 2014.

13) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Effects of Organic Ligands on the Optical Properties of Undecagold Nanoclusters,* XXV Congress SCI, Rende (Italy), September 2014.

14) **F. Muniz-Miranda***, M. C. Menziani, A. Pedone, *Simulating Ag-based nanoclusters at the quantum-chemical level*, 7th International Conference of Molecular Electronics (Elecmol7), Strasbourg (France), August 2014.

15) **F. Muniz-Miranda**, M. C. Menziani, A. Pedone, *Effects of Organic Ligands on the Optical Properties of Undecagold Nanoclusters*, 7th International Conference of Molecular Electronics (Elecmol7), Strasbourg (France), August 2014.

16) **F. Muniz-Miranda***, M. C. Menziani, A. Pedone, "*Ab initio Investigation of a Gold Nanocluster: is the Optical Spectrum due to Ligands?"*, Winter Modelling 2014, Modena (Italy), March 2014.

17) **F. Muniz-Miranda***, M. C. Menziani, A. Pedone, *DFT Strategies to Approach Gold and Silver Nanoclusters*, 2nd Avogadro Colloquia, Scuola Normale Superiore, Pisa (Italy), September 2013. Video: https://www.youtube.com/watch?v=u17McGXJ98E

18) R. Righini, **F. Muniz-Miranda**, R. Chelli, V. Volkov, *Structure and dynamics of a membrane associated anchor dipeptide*, Second International Conference on «Transient Chemical Structures in Dense Media», Paris (France), November-December 2011.

19) M. Pagliai, **F. Muniz-Miranda**, V. Schettino, M. Muniz-Miranda, *Competitive Solvation and Chemisorption in Silver Colloidal Suspensions,* UK Colloids Conference, London (U.K.), July 2011.

20) **F. Muniz-Miranda***, M. Pagliai, G. Cardini, R. Righini, V. Schettino, *Spectroscopic properties of hydrogen bonded systems by wavelet analysis*, XXX EUCMOS (European Congress of Molecular Spectroscopy), Florence (Italy), August-September 2010.

21) M. Pagliai, **F. Muniz-Miranda**, G. Cardini, R. Righini, V. Schettino, *Hydrogen bond dynamics of methyl acetate in methanol*, XXX EUCMOS (European Congress of Molecular Spectroscopy), Florence (Italy), August-September 2010.

***** = (**presenting author**)

Research databases:

Research Gate profile:
https://www.researchgate.net/profile/Francesco_Muniz-Miranda
Google Scholar profile:
https://scholar.google.it/citations?user=puaMVcEAAAAJ&hl=it
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Suggested contacts/referees:

Prof. Dr. **Carlo Adamo** (chaired full professor at the Chimie ParisTech)
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Dr. **Ilaria Ciofini** (research director at the French CNRS)
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Prof. Dr. **Gianni Cardini** (full professor, UniFI)
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Prof. Dr. **Roberto Righini** (emeritus full professor, LENS)
- righini@lens.unifi.it

Prof. Dr. **Alfonso Pedone** (associate professor, UniMORE)
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Prof. Dr. **Veronique Van Speybroeck** (full professor, UGent)
- veronique.vanspeybroeck@ugent.be

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Articles, book chapters, etc…

1) **F. Muniz-Miranda,** *Computational approaches to the electronic properties of noble metal nanoclusters protected by organic ligands, 2021,* Nanomaterials **2021**, 11(9), 2409

2) 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**, 2000426 (pp. 1-8), Doi: 10.1002/marc.202000426

3) 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

4) 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

5) 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

6) 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

7) 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

8) **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

9) 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

10) 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

11) **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

12) 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

13) 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

14) 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

15) **F. Muniz-Miranda**, *Metal Clusters: a TD-DFT Study* (*Cluster Metallici: uno studio TD-DFT*), La Chimica & L'Industria, Anno II, N. 3 – Maggio/Giugno 2019, pp. 62-64, ISSN: 2283-5458, http://dx.medra.org/10.17374/CI.2019.101.3.67

16) 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

17) **F. Muniz-Miranda** (corresponding), 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

18) 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

19) 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

20) 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

21) **F. Muniz-Miranda** (corresponding), 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

22) M. Muniz-Miranda, **F. Muniz-Miranda**, A. Pedone, *Spectroscopic and computational studies on ligand-capped metal nanoparticles and clusters,* in "Metal Nanoparticles and Clusters", Deepak, Francis Leonard (Ed.), Springer Series in Materials Science, Springer International Publishing, Switzerland, ISBN: 978-3-319-68052-1, Doi: 10.1007/978-3-319-68053-8_3, Chapter 3, pp. 55-87, **2017**

23) 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

24) **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

25) 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

26) **F. Muniz-Miranda** (corresponding), 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

27) 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

28) **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

29) **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

30) **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

31) **F. Muniz-Miranda** (corresponding), 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

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