Univ.-Prof. Dr. Dr. h.c. Leticia González

Academic CV and description of previous research achievements

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Academic milestones and positions held to date

2017-2021	Spokewoman of the Arbeitsgemeinschaft Theoretische Chemie
since 2011	Full Professor for Computational Chemistry, Theoretical Chemistry and Scientific Computing at the Institut für Theoretische Chemie, Faculty of Chemistry, Universität Wien
2007-2011	W2-Professor for Physical and Theoretical Chemistry at the Friedrich-Schiller-Universität Jena
2007	Heisenberg Fellow at the Department of Chemistry, Freie Universität Berlin
1999-2006	Assistant Professor at the Department of Chemistry, Freie Universität Berlin
2005	Venia Docendi in Theoretical Chemistry, Freie Universität Berlin
2004	Habilitation in Theoretical Chemistry, Freie Universität Berlin
1998	Ph.D. in Chemistry ("Premio Extraordinario")
1995-1998	PhD student with O. Mó and M. Yáñez, Universidad Autónoma de Madrid
1995	MSc thesis with M. A. Robb at King´s College London
1989-1994	Chemistry studies ("Licenciatura") at Universidad Autónoma de Madrid

Main areas of research and short statement of the most important results

We investigate chemical and photochemical phenomena using state-of-the-art electronic structure methods and reaction dynamics techniques. In particular, we have made substantial contributions to the field of photochemistry, non-adiabatic dynamics and computational spectroscopy. We have developed a general code (SHARC) to describe excited state dynamics in the presence of any arbitrary coupling, such as kinetic, spin-orbit and dipole couplings. This allowed us to investigate DNA building blocks, transition metal complexes and small to medium organic molecules, in gas phase or in the presence of complex environments. In the latter case, we make use of multiscale methods, such as QM/MM.

Most important scientific and scholarly results achieved to date:

- Almost 300 peer-review publications with ~9000 citations, h-Index 46(WoS) /53(GoogleS), i10=195
- Co-editor of 6 thematic special issues, 17 book chapters, and 1 book
- Reviewer for Nature Chemistry, Nature Communications, PNAS, Chemical Science, Angewandte Chemie, J. Am. Chem. Soc., J. Phys. Chem. Lett., among many others.
- Editorial Advisory Board of Chemical Science, J. Phys. Chem. Lett., J. Am. Chem. Soc. Au, and Angewandte Chemie.

- Editorial member of ChemPhysChem (Wiley), ChemPhotoChem (Wiley), Chemical Physics Letters (Elsevier), Theoretical Chemical Accounts (Springer) and Chemical Monthly (Springer)
- Reviewer for the European Union (ERCs), the National Science Foundation, the Swiss National Science Foundation, the French National Agency of Research, the Austrian Ministry of Science, Research and Economy (BMWFW), the Max Planck Society, the University of Vienna, and the German Science Foundation (DFG), the latter including review panels for collaboratory SFBs, GKs and TRRs.
- Member of the Expert Panel at the Joint Science Conference (GWK), German Research Council
- Member of the Scientific Advisory Board at the Max Planck Institute for Coal Research in Mülheim/Ruhr, at the J. Heyrovsky Institute of Physical Chemistry of the CAS in Prague and at the Institute for Advance Research in Chemical Sciences, Universidad Autónoma de Madrid
- More than 200 Invited talks (>100 Plenary lectures) at conferences, international and national institutions, e.g. plenary lectures at the Gordon Research Conferences (GRC) on "Atomic and Molecular Interactions" 2010, on "Electronic Spectroscopy and Dynamics" 2012, on "Quantum Control of Light and Matter" 2013, on "Photochemistry" 2013, on "Molecular Interactions and Dynamics" 2016, on "Gaseous Ions: Structures, Energetics, and Reactions" 2019, WATOC, ICQC, etc.
- Home of the SHARC software code for molecular dynamics, www.sharc-md.org
- Pioneering surface-hopping studies on intersystem crossing dynamics with unprecedented ultrafast time scales
- First excited state dynamics studies in full dimensionality in transition metal complexes
- Quantification of delocalization in DNA using multiscale techniques

Top 10 academic publications

1. C. Daniel, J. Full, L. González, C. Lupulescu, J. Manz, A. Merli, S. Vajda, L. Wöste
   Deciphering the reaction dynamics underlying optimal control laser fields
   Science **2003**, *299*, 536-539, DOI: 10.1126/science.1078517
2. L. González, D. Escudero, L. Serrano-Andres
   Progress and challenges in the calculation of electronic excited states
   ChemPhysChem **2012,** *13*, 28-51 DOI: 10.1002/cphc.201100200
3. M. Richter, P. Marquetand, J. González-Vázquez, I. Sola, L. González
   SHARC - *ab initio* molecular dynamics with surface hopping in the adiabatic representation including arbitrary couplings
   J. Chem. Theory Comput. **2011,** *7*, 1253-1258 DOI: 10.1021/ct1007394
4. S. Tschierlei, M. Karnahl, M. Presselt, B. Dietzek, J. Guthmuller, L. González, M. Schmitt, S. Rau, J. Popp
   Photochemical fate: The first step determines efficiency of H_2 formation with a supramolecular photocatalyst
   Angew. Chem. Int. Ed. 49, 3981-3984, (2010), DOI: 10.1002/anie.200906595
5 J. P. Zobel, J. J. Nogueira, L. González
   The IPEA dilemma in CASPT2
   Chem. Sci. **2017.** *8*, 1482-1499 DOI: 10.1039/C6SC03759C
6. S. Mai, N. Dunn, L. Martinez-Fernandez, M. Pollum, P. Marquetand, I. Corral, C. Crespo-Hernández, L. González
   The origin of efficient triplet state population in sulfur-substituted nucleobases
   Nat. Commun. **2016**, 7, 13077, DOI: 10.1038/ncomms13077

7. S. Mai, P. Marquetand, L. González
   Nonadiabatic dynamics: The SHARC approach
   *Wiley Interdiscip. Rev. Comput. Mol. Sci.***2018,** 8, e1370, DOI: 10.1002/wcms.1370
8. F. Plasser, M. Ruckenbauer, S. Mai, M. Oppel, P. Marquetand, L. González
   Efficient and flexible computation of many-electron wavefunction overlaps
   J. Chem. Theory Comput. **2016,** 12, 1207-1219, DOI: 10.1021/acs.jctc.5b01148
9. A. J. Atkins, L. González
   Trajectory surface-hopping dynamics including intersystem crossing in $[Ru(bpy)_3]^{2+}$
   J. Phys. Chem. Lett. **2017,** 8, 3840-3845, DOI: 10.1021/acs.jpclett.7b01479
10. J. J. Nogueira, F. Plasser, L. González
    Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis
    Chem. Sci. **2017,** 8, 5682-5691, DOI: 10.1039/C7SC01600J

Additional research achievements

2020-2023	Principal Investigator of the DFG/FWF, Transregio (SFB/TRR) 234: "Light-driven Molecular Catalysts in Hierarchically Structured Materials – Synthesis and Mechanistic Studies", PI Budget 398k€
2020-2024	Coordinator of the “Vienna Research Platform on Accelerating Photoreaction Discovery (ViRAPID)”, funded by the University of Vienna, total budget 550k€
2019	Robert Bunsen-Lecture Prize, DBG (German Bunsen Society)
2019	Elected Member of the Austrian Academy of Sciences (ÖAW)
2019	Prize for Excellent Research from the Spanish Royal Society of Chemistry
2019	Fellow of the European Academy of Sciences (EurASc)
2018	Gauß-Professorship, Göttingen Academy of Sciences and Humanities; Doctor Honoris Causa award of the Université de Lorraine, France; ChemPubSoc Europe Fellow (Class 2016/2017)
2014	Löwdin Lecture, Uppsala Universitet, Sweden
2011	Dirac Medal from the World Association of Theoretical and Computational Chemists
2005	SIGMA-ALDRICH Young Investigator Award, Spanish Royal Society of Chemistry