Curriculum Vitae (Scientific)

TERENCIO Thibault

Gender : **M** Age : **35**

Present time

Teacher-Researcher at Yachay Tech University from 01/12/17 to present time

University degrees

PhD	**Theoretical chemistry, dual theory-experience**	-2013 (ENSCM Montpellier)
Master degree	**Theoretical chemical physics**	-2010 (UPS Toulouse)
License degree	**Molecular chemistry**	-2009(UPS Toulouse)

Language

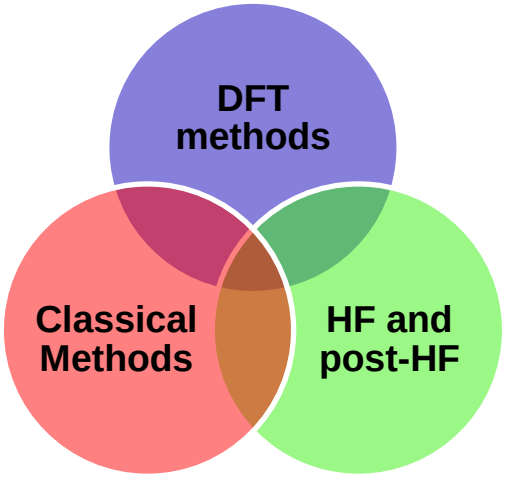
French	**native speaker**	Spanish	**fluent**
English	**fluent**	German	**basic level** (from high-school)

General scientific profile

Main scientific domains:

Theory, catalysis, spectroscopy, materials, excited states

Competences in theoretical chemistry



DFT methods	Geometry optimizations, calculation of vibration frequencies, charges, localized orbitals, transition states, TD-DFT… Calculation including dispersion forces (DFT+D)
Classical methods (Monte-Carlo, molecular dynamics)	Simulation of adsorption isotherms Simulation of XRD spectra Calculation of adsorption enthalpies Configurationnal-Bias Monte Carlo (CBMC)
HF and post-HF methods (IC, CASPT2)	Study of magnetic and mixed valence compounds Deep analysis of wave-function: extraction of microscopic parameters (J,t,U,K), model Hamiltonians (Heisenberg, t-J, Hubbard)

Competences in informatics

General knowledge

- Windows/Linux environment
- Programming in different languages: python, perl, FORTRAN, C, bash script, html, php, C++,
- Matlab, Qt, visual basic...
- Data treatment and file conversion (perl/python)
- Programming of micro-controllers (Arduino)
- 3D printing, 3D modelling
- Other software: Excel, Origin...

Specific knowledge

- Calculation programs used: Orca, Gaussian, VASP, Molcas, Casdi, Towhee, DLPOLY,
- Hyperchem, Material Studio modules
- Calculation on big clusters with queue system (CINES, Quinde I)
- Visualization programs used: VMD, Avogadro, Mercury, Molden, Material Studio, gaussview
- 3D modelisation/graphism: pov-Ray, cinéma 4D, blender, CorelDraw, Photoshop, GIMP, After Effects, FreeCad...

Competences in experimental chemistry

IR Spectroscopy, Diffuse reflectance IR (DRIFT), UV spectroscopy, diffuse reflectance UV (DRUV), ATG, Gravimetry, nitrogen adsorption and analysis, Mass spectrometry, with ion trapping and collision induced dissociation, Interpretation of Infrared multi-photon dissociation, near-IR.

Engineering of experimental device for studying adsorption by IR measurement in-situ during PhD. This required to make a plan of it and taking into consideration all the different requirements, length of tubes, pressure, material of tubes (resisting to gas acetone)... The apparatus allowed to record the adsorption at very low partial pressure of acetone.)

Systems and analysis achieved

Systems studied

Big scale systems (>150 atom), hybrid systems (organic and inorganic)
System with complex electronic structure: magnetic, mixed valence compounds, uranium
Interchange from one scale to another (classic -> non periodic DFT -> periodic DFT)

Analysis

Conformational analysis, uncovering interaction nature between adsorbate and adsorbent, Analysis of position of adsorption sites, Analysis of wave-function in order to extract microscopic parameters (J, t...), Modelisation (Heisenberg, t-J), Unrevealing reactions mechanisms, transition states search, Luminescence calculations.

Research Experiences

Research: internships master1+master2

Supervisors: N. Guihéry, J-P Malrieu, N. Suaud *3 + 5 months,*

Subject: Study of microscopic mechanisms under magnetic coupling in bi-centric systems.

Generalized Anderson mechanism should predict, in bi-metallic systems, the magnetic behavior. However, the experiments conducted by J. Bonvoisin contradicted this prediction. Another mechanism, different from Anderson, was then evocated in order to explain that deviation: spin polarization. Thanks to a program I developed, we could separate these 2 mechanisms, and then show that spin polarization is predominant at long range distance.

Research: PhD

Supervisors: P. Trens, D.Berthomieu, F. Di Renzo *3 years,*

Subject: Study of VOCs adsorption on MOFs by a dual theoretical-experimental approach.

Volatile Organic Compounds (VOCs) are massively produced each day, and contribute strongly to the degradation of the quality of life.

Adsorption is a simple process which allows further re-use of captured compounds. In this PhD, we studied Metal Organic Frameworks (MOFs) as potential new adsorbents. MOFs are materials constituted of both organic and inorganic parts which can be precisely modulated through a design process.

The main objective of this work was to give insights about microscopic interaction controlling adsorption phenomena of VOCs in MOFs.

Through classical approach, this study showed the behavior of linear alkanes adsorbed inside three different MOFs (MIL-47, MIL-125 et UiO-66) highlighting the importance of shape porosity and alkane folding.

Other part of this study was also about the behavior of a polar molecule, acetone, inside Cu-BTC. The *in-situ* IR study, compared to quantum approach, allowed to make a link between the frequency of C=O stretching of acetone and the position of this molecule inside the MOF and to highlight that it is a limit case between a preferential adsorption driven by electronic forces at Lewis acid sites and by VdW forces inside a cage.

Research: Post-doctoral

Supervisor: J. Roithova *2 years,*

Study elementary steps in organic and organometallic reactions using mass spectrometry, ion spectroscopy and quantum chemistry. The aim is a deeper understanding of reaction mechanisms and formulation of new general concepts in organic and organometallic reactivity.

Research: Teacher-researcher (present time)

Founder of CATS (Catalysis, Theory and Spectroscopy) research group *3 years-,*

My research is focused in different fields, mainly in theoretical chemistry, following my previous experiences in magnetism, materials and catalysis but expanding also to luminescent properties or biological activities among others.

Teaching experience:

PhD: Teaching assistant

At the chemical engineer school ENSCM *3 years (During PhD)*

Topics:

- Theoretical chemistry (Classic and quantum)
- Informatics (Visual Basic and Access)

Teacher-researcher (Yachay):

At Yachay Tech University 12/2017-now

Topics:

- Introduction to computational chemistry (theory and laboratory)
- Chemistry I (laboratory)
- Chemistry II (laboratory)
- GAR of chemistry (preparation course for best high-school students at university entrance)
- Informatics applied to chemistry (theory and laboratory)
- Chemistry I (Theory) for students from ECE UNAE
- DFT applied to chemistry (theory/lab)
- Computational physics (theory/lab)

Other activities:

- Student's leader during PhD
- Founder and director of a research group (Catalysis Theory and Spectroscopy - CATS)
- Member of the commission in charge of constituting a master program in chemistry (part of theoretical chemistry speciality)
- Member of the sub-commission of evaluation of contestation in concourses for permanent professors
- Formations for upgrading communication skills
- Jury of undergraduates tesis
- Jury of poster selection
- Jury for pre-selection in summer school
- Article reviewer
- Advisor for French language club "La mouche a feu"
- Responsible for teaching and researching assistants
- Organizer of local event with international gues (CATS special guests)
- Tutor in Vinculation projects

Scientific production

Publication (11)

Data Scopus: h-index: 7, citations: 133, publications Q1: 11

Data Google scholar: h-index: 7, i-10 index: 6, citations: 162

- "Physical analysis of the through-ligand long-distance magnetic coupling: spin-polarization *versus* Anderson mechanism", *phys. Chem. chem. phys.*, **T. Terencio ; R. Bastardis ; N. Suaud ; D. Maynau ; J. Bonvoisin ; J. P. Malrieu ; C. J. Calzado ; N. Guihéry*** (2011) https://doi.org/10.1039/C1CP20179D

- "The Adsorption of Acetone Vapour by Cu-BTC: A Combined Experimental and Theoretical Investigation", *J. Phys. Chem. C*, **T. Terencio ; F. Di Renzo ; D. Berthomieu ; P. Trens*** (2013) https://doi.org/10.1021/jp410152p

- "Chasing the Evasive Fe═O Stretch and the Spin State of the Iron(IV)–Oxo Complexes by Photodissociation Spectroscopy", *J. Am. Chem. Soc.*, **Erik Andris ; Rafael Navrátil ; Juraj Jašík ; Thibault Terencio ; Martin Srnec* ; Miquel Costas* ; Jana Roithová*** (2017) https://doi.org/10.1021/jacs.6b12291

- "Palladium catalyzed C–H activation: Mass spectrometric approach to reaction kinetics in solution.", Organomettalics, **Jiří Váňa ; Vladimir Petrović ; Thibault Terencio ; Orsolya Tischler ; Zoltán Novák ; Jana Roithová*** (2017) https://doi.org/10.1021/acs.organomet.6b00960

- "A Comparative IRMPD and DFT Study of Fe^{3+} and UO_2^{2+} Complexation with N-Methylacetohydroxamic Acid",Inorg. Chem., **Thibault Terencio ; Jana Roithová* ; Stéphane Brandès ; Pawel Jewula ; Jean-Claude Chambron ; Michel Meyer*** (2018) https://doi.org/10.1021/acs.inorgchem.7b02567

- "Chemoselectivity in the Oxidation of Cycloalkenes with a Non-Heme Iron(IV)-Oxo-Chloride Complex: Epoxidation vs. Hydroxylation Selectivity", J. Am. Soc. Mass Spectrom., **Thibault Terencio ; Erik Andris ; Martin Srnec ; Miquel Costas ; Jana Roithova** (2019) https://doi.org/10.1021/jasms.8b06213

- "Sugar-Mediated Green Synthesis of Silver Selenide Semiconductor Nanocrystals under Ultrasound Irradiation", Molecules, **García, D.A.*; Mendoza, L.; Vizuete, K.; Debut, A.; Arias, M.T.; Gavilanes, A.; Terencio, T.; Ávila, E.; Jeffryes, C.; Dahoumane, S.A.*** (2020) https://doi.org/10.3390/molecules25215193

- "A Theoretical and Experimental Study on the Potential Luminescent and Biological Activities of Diaminodicyanoquinodimethane Derivatives", International Journal of Molecular Science, **Edison Rafael Jiménez ; Manuel Caetano ; Nelson Santiago ; F. Javier**

Torres ; Thibault Terencio* ; Hortensia Rodríguez* (2021) https://doi.org/10.3390/ijms22010446

- "Polytetrafluoroethylene-like Nanoparticles as a Promising Contrast Agent for Dual Modal Ultrasound and X-ray Bioimaging", ACS Biomaterials Science & Engineering, **Cristhian Marcelo, Chingo Aimacaña; Dilan Andres, Quinchiguango Perez; Suyene Rocha Pinto; Alexis Debut; Mohamed F. Attia; Ralph Santos-Oliveira; Daniel C. Whitehead; Thibault Terencio; Frank Alexis*; Si Amar Dahoumane*** (2021) https://doi.org/10.1021/acsbiomaterials.0c01635

- "Biogenic Sulfur-Based Chalcogenide Nanocrystals: Methods of Fabrication, Mechanistic Aspects, and Bio-Applications" Molecules 27 (2), 458, **Oscar P Yanchatuña Aguayo, Lynda Mouheb, Katherine Villota Revelo, Paola A Vásquez-Ucho, Prasad P Pawar, Ashiqur Rahman, Clayton Jeffryes, Thibault Terencio*, Si Amar Dahoumane* (2021)**

- "Delta Chem: A New Geometric Approach of Porosity for Symmetric Porous Materials", Journal of Chemical Information and Modeling **, JL Castro Angamarca, R Manzanilla Morillo, T Terencio*** (2022)

Publication – other contribution

Mariarosa Anania ; Lucie Jasikova ; Juraj Jasik ; Jana Roithová, "Why can a gold salt react as a base?", Org. Biomol. Chem., 2017, 15, 7841-7852 (in acknowledgement section for theoretical calculations)

Congress participation (only presented)

- "Adsorption of acetone on Cu-BTC", **T. Terencio et al. ,** *Calorimetry and Thermal Effects in Catalysis*, June 28, 2012 (oral)

- "Epoxidation over Hydroxylation selectivity of cycloalkenes with an iron(IV)-oxo complex. What factors influence it?", **T. Terencio et al.**, *Liblice 2016: Advances in Organic, Bioorganic and Pharmaceutical Chemistry*, Lázně Bělohrad, November 11-13, 2016 (oral)

- "Comparative study of UO_2^{2+} and Fe^{3+} complexation with hydroxamate siderophore", **T. Terencio et al.**, *5th Conference of the Czech Society for Mass Spectrometry*, České Budějovice, Czech Republic, April 13-15, 2016 (oral)

- "Comparative study of UO_2^{2+} and Fe^{3+} complexation with hydroxamate siderophore", **T. Terencio et al.**, *7th French-Czech "Vltava" Chemistry Meeting*, Orléans, France, September 4-7, 2016 (oral)

- "Theoretical chemistry at Yachay Tech", **T.Terencio**, Humboldt Kolleg, 2019 (poster)

- "A geometric approach of porosity: Development of DeltaChem, a new algorithm for finding adsorption sites in porous materials" Jorge Castro, Raúl Manzanilla, Thibault Terencio, VII REDU congress 2019 (poster)

- "Chemoselectivity in the oxidation of cycloalkenes with a non-heme Iron(IV)-oxo-chloride complex: Epoxidation vs. hydroxylation selectrivity", **T.Terencio**, CTTC (Current Topics in Theoretical Chemistry workshop), 2019 (oral)

- "De la estructura electronica hasta el mundo macro: Los electrones definen la química?", **T.Terencio**, IST 17 de Julio, 2019 (oral)

- "Theoretical and computational chemistry at Yachay Tech", **T.Terencio**, Webinar Yachay Tech, 2020 (oral virtual)

- "La química teórica en el campo profesional", **T.Terencio**, IST 17 de Julio, 2020 (oral)

- "CATS perspectives in chemistry", **T.Terencio**, Yachay Tech, 2021 (oral)

Student work direction (tutor or cotutor)

Undergraduate thesis: 15 directions – Undergraduate thesis are one year long

These works are consultable in https://repositorio.yachaytech.edu.ec/simple-search?query=terencio

- **Jeremee Zenteno**, (2019), tutor, "NI-DOPED CU-BTC FOR DIRECT HYDROXYLATION OF BENZENE TO PHENOL"
  Current results: 2 poster presentations, 1 poster prize

- **Jorge Castro**, (2020), tutor, "A geometric approach of porosity: development of Delta Chem, a new software for finding adsorption sites in microporous materials"
  Current results: 2 presentations

- **Rafael Jimenez**, (2020), co-tutor, "An experimental and theoretical approach to diaminodicyanoquinodimethanes derivatives with luminescent and biological activities"

- **Jose Andino**, (2020), co-tutor, "Orbital coupling and dependence of mechanical deformation in molecular structures"

- **Adrian Muriel**, (2020), tutor, "alkanes diffusion through punctually modified nanotubes"

- **Alexander Tipan**, (2020), co-tutor, "Possibility of Reusing industrial waste to synthesize a depolluting silica monolith through HIPE method: an experimental and theoretical study"

- **Paula Cardenas**, (2020), tutor, "Theoretical study on the Photoactivated anticancer drugs based on platinum coordination compounds"

- **Joselyn Delgado**, (2020), co-tutor, "A dual experimental-theoretical approac h to the spectroscopic properties of lignin originating from rose stems"

- **Carlos Michael Jimenez Muñoz**, (2021), tutor, "A dual theoretical-experimental study of Iron complexing with N-ligand: understand and design a catalyst", *ongoing*

- **Alexander Ricardo Riascos Flores**, (2021), tutor, "Sandwich monoliths", *ongoing*

- **Jorge Humberto Chavez Ruiz**, (2021), tutor, "How to make an eco-friendly and unlimited printer?", *ongoing*

- **Alexander Eduardo Escobar Pullas**, (2021), tutor, "MODELLING OF COORDINATION POLYMER OF POLYMER OF M2+ (M = ZN, CO, CU) FROM DITOPIC ORGANIC LINKERS (MALEIC ACID, 1,2-DICARBOXYLIC-BENCENE ACID AND 4,4'-BIPYRIDINE) AND THEIR PHOTOREACTIVE PROPERTIES", *ongoing*

- **Henry Bryan Romero Lopez**, (2021), co-tutor, "Kinetical models for facultative bacteria Cupriavidus Necator behavior on oil degradation from comestible oil wastewater industry", *ongoing*

- **Maria Emilia Iglesias Moncayo**, (2021), co-tutor, "SPECTROSCOPIC AND REDOX PROPERTIES OF BIOMIMETICS OF COPPER METALLOPROTEINS: A PRACTICAL AND THEORETICAL APPROACH"

- **Oscar Patricio Yanchatuña Aguayo**, (2021), tutor, "Biogenic sulfur-based nanocrystals: methods of fabrication and applications"

Projects

- **Automatización para la cristalografía**, Principal Researcher, YachayTech, 01/01/2019-30/06/2020

- **Utilización y modificación de los Metal Organic Framework (MOF) para la catálisis,** Principal Researcher, YachayTech, 01/08/2018-31/12/2019

- **Estudio de catalizadores de hierro**, Principal Researcher, YachayTech, 01/01/2018-31/12/2019

- **Modelo teórico de la difusión en los nanotubos de carbono**, Principal Researcher, YachayTech, 01/01/2019-30/09/2020

- **Los monolitos sanduches, un nuevo tipo de material multifuncional,** Principal Researcher, YachayTech, 22/09/2021-

- **Estudio teórico de los efectos geométricos del ámbito cercano de los enlaces hidrógenos y su efecto en la interacción con la luz,** Principal Researcher, YachayTech, 22/09/2021-

- **BIOFe: Biochar derivado de residuos de guadua angustifolia dopado con Fe para la eliminación de Pb, As y Cd en aguas de la Amazonía ecuatoriana mediante procesos de adsorción y digestión anaerobia. BIOFE AGUAS AMOZONIA.,** collaborator, convocatoria CEPRA XVI-2022-13-

- **Preparación de nanostructuras carbonáceas luminiscentes a partir de biomasa extraida de desechos agrícolas,** collaborator, YachayTech

- **Bio-adsorbentesde bajo costopara la remoción desustanciastóxicas de aguas residuales y de riego,** collaborator, YachayTech

- **Preparación de nanopartículas metálicas funcionalizadas a partir de componentes de biomasa,** collaborator, YachayTech

Awards and acknowledgments

- Ackowledgement best professor
- Ackowledgement best thesis tutor
- 1st place during the poster session 1 on May 28, 2019, SCHOOL OF PHYSICAL SCIENCES AND NANOTECHNOLOGY, Jeremee Zenteno (thesis student)
- 7-8 septiembre de 2020. "#LatinXChem Twitter Conference 2020 on Sept 7th 2020 " organizado por LATINXCHEMSA, USA. (póster trabajo Nadia López, primer lugar mejor póster en la categoría).