Maxime Ferrer | Ph. D.

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Education

Postdoctoral Contrat in Machine Learning applied to Chemistry — **Paris, France**
Ecole Normale de Chimie Paris – PSL, Supervisor: Thijs Stuyver — 2024-...

International PhD in Theoretical Chemistry and Computational Modelling — **Madrid, Spain**
2020-2024
Instituto de Química Médica – CSIC, supervisors: Prof Ibon Alkorta, Dr. Josep Oliva-Enrich
Title: Exploring the mechanisms of CO_2 capture by intramolecular Frustrated Lewis Pairs. – Defended 04/10/2024.

M. Sc. Theoretical Chemistry and Computational Modelling — **Madrid, Spain**
University Autonomous of Madrid, supervisors: Dr. Ma Merced Montero-Campillo, Dr. Julia Contreras-García — 2018-2020

B. Sc. in Chemistry — **Toulouse, France**
University Toulouse III – Paul Sabatier — 2015-2018

Internships

Univeristy of Manchester — **Manchester, UK**
Supervisor: Dr. Cristina Trujillo — 2023

Trinitiy College Dublin — **Dublin, Ireland**
Supervisor: Dr. Cristina Trujillo — 2022

Sorbonne University — **Paris, France**
Supervisor: Dr. Julia Contreras-García — 2020

University of British Colombia — **Vancouver, Canada**
Supervisor: Dr. Pierre Kennepohl — 2018

Scientific Summary

Articles: 23
H-index: 6
Citations: 94
ORCID: 0000-0001-7838-9974

Research experience

Computational Chemistry
Molecular Structure, non-covalent interactions, aromaticity
DFT, MP2 methods, electron density analysis (AIM), NBO, ELF, MEP, EDA, GIAO, NICS, EDS

Computational Chemistry
Development of methods
Programming in Fortran90, Python, basis in Machine Learning

Publications

[23] **Maxime Ferrer**, José Elguero, Ibon Alkorta, Luis Miguel Azofra, *Understanding the coupling of non-metallic heteroatoms to CO2 from a Conceptual DFT perspective*, **2024**, 30(7), 201

[22] Iñigo Iribarren, **Maxime Ferrer**, Ibon Alkorta, Cristina Trujillo, *Computational Insights into Cinchona-Based Phase Transfer Catalysis for Asymmetric Conjugate Cyanation*, Eur J. Org. Chem, **2024**, e202400329

[21] Josep M. Oliva-Enrich, **Maxime Ferrer**, Ibon Alkorta, José Elguero, Julio Barrios, William Tiznado, *Striking Borane Planarization in the Thermal Rearrangement (η5-C5H5)Fe(η3-B5H10) → (η5-C5H5)Fe(η5-B5H10)*, ChemEurJ, **2024**, e202401536

[20] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *A multi-FLP approach for CO2 capture: investigating nitrogen, boron, phosphorus and aluminium doped nanographenes and the influence of a sodium cation*, PCCP, **2024**, 26, 12433

[19] **Maxime Ferrer,** Ibon Alkorta, José Elguero, *Theoretical study of the formation of pyrazole and indazole carbamic acids,* Struct Chem, **2024**, 35, 393

[18] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *Capture of CO_2 by Melamine Derivatives: A DFT Study Combining the Relative Energy Gradient Method with an Interaction Energy Partitioning Scheme*, J. Phys. Chem. A, **2024**, 128, 7, 1288

[17] Rubén López-Sánchez, **Maxime Ferrer**, Josep M. Oliva-Enrich, Ibon Alkorta, José Elguero, *Towards 2D Borane Chemistry in Hexagonal Cyclic Compounds*, ChemPhysChem, **2024**, 25, e202300809

[16] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *(Pyridin-2-ylmethyl)triel Derivatives as Masked Frustrated Lewis Pairs. Interactions and CO_2-Sequestration*, ChemPhysChem, **2024**, 25, e202300750

[15] Majid Rezaeivala, Hassan Keypour, Sareh Tamizi, Hojatollah Fatemikia, Ibon Alkorta, **Maxime Ferrer**, Robert William Gable, *Synthesis and characterization of two novel fused macrocyclic ligands: Experimental and theoretical studies*, J. Mol. Struct., **2023**, 1290, 135936

[14] Ofelia B. Oña, **Maxime Ferrer**, Diego R. Alcoba, Alicia Torre, Luis Lain, Gustavo E. Massaccesi, Douglas J. Klein, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *A quantum-chemical study of boro-fullerenes $B_{60}H_{60}$, $B_{60}F_{30}H_{30}$, and $B_{60}F_{60}$,* Comp Theo Chem, **2023**, 1220, 113987

[13] Marta Delgado Gómez, Dr. Marco Marazzi, Prof. José Elguero, **Maxime Ferrer**, Prof. Ibon Alkorta, *Production of Dihydrogen Using Ammonia Borane as Reagent and Pyrazole as Catalyst*, ChemPhysChem, **2023**, 24, e202300214

[12] José F. Marco, Juan Z. Dávalos-Prado, Drahomír Hnyk, Josef Holub, Ofelia B. Oña, Diego R. Alcoba, **Maxime Ferrer**, José Elguero, Luis Lain, Alicia Torre, and Josep M. Oliva-Enrich, *Two Shared Icosahedral Metallacarboranes through Iron: A Joint Experimental and Theoretical Refinement of Mössbauer Spectrum in [Fe(1,2-$C_2B_9H_{11})_2$]Cs,* ACS Omega, **2023**, 8, 15, 13993

[11] Carlos Martín-Fernández, **Maxime Ferrer**, Ibon Alkorta, Merced Montero-Campillo, José Elguero, Marcos Mandado, *Metastable Charged Dimers in Organometallic Species: A Look into Hydrogen Bonding between Metallocene Derivatives*, Inorg. Chem., **2023**, 62, 40, 16523

[10] **Maxime Ferrer**, Ibon Alkorta, Josep M. Oliva-Enrich, José Elguero, *Borane derivatives of five-membered N-heterocyclic rings as frustrated Lewis pairs: activation of CO_2,* Struct Chem, **2023**, 34, 1591

[9] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *A theoretical study of the reaction of borata derivatives of benzene, anthracene and pentacene with CO_2,* Phys Chem Chem Phys, **2023**, 25, 22512

[8] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *Reactivity of a model of B_3P_3-doped nanographene with up to three CO_2 molecules,* Sci. Rep, **2023**, 13, 2407

[7] Laimutis Bytautas, Douglas J. Klein, Demeter Tzeli, **Maxime Ferrer**, José Elguero, Ibon Alkorta, Josep M. Oliva-Enrich, *Chapter 6: Progress in Electronic-Structure Based Computational Methods: From Small Molecules to Large Moleculer Systems of Biological Significance*, Frontiers in Computational Chemistry, **2022**, Vol 6., 235

[6] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *Use of 5,10-Disubstituted Dibenzoazaborines and Dibenzophosphaborines as Cyclic Supports of Frustrated Lewis Pairs for the Capture of CO_2,* ChemPhysChem, **2022**, 23, e202200204

[5] Douglas J. Klein, **Maxime Ferrer**, José Elguero, Laimutis Bytautas, Josep M. Oliva-Enrich, *Hückeloid model for planar boranes*, Theor Chem Acc, **2021**, 140, 55

[4] Josep M. Oliva-Enrich, Ibon Alkorta, José Elguero, **Maxime Ferrer**, José I. Burgos, *On the 3D → 2D Isomerization of Hexaborane(12*), Chemistry, **2021**, 3, 1, 28

[3] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *Carboranes as Lewis Acids: Tetrel Bonding in $CB_{11}H_{11}$ Carbonium Ylide,* Crystals, **2021**, 11. 4. 391

[2] **Maxime Ferrer**, Ibon Alkorta, José Elguero, Josep M. Oliva-Enrich, *Sequestration of Carbon Dioxide with Frustrated Lewis Pairs Based on N-Heterocycles with Silane/Germane Groups*, J. Phys. Chem. A, **2021**, 125, 32, 6976

[1] **Maxime Ferrer**, M. Merced Montero-Campillo, Otilia Mó, Manuel Yáñez, Ibon Alkorta, José Elguero, *Bonding between electron-deficient atoms: strong Lewis-acid carácter preserved in X-Y-X (X=B, Al; Y=Be, Mg) bridges*, New. J. Chem, **2020**, 44, 11870