CNRS THEMATIC SCHOOL MODERM

4-7 September 2023

WELCOME BOOK

https://moderm2023.sciencesconf.org/

Welcome Letter

The electron density analyses allow to rationalize the quantum computations in chemical terms such as bonds, lone pairs, electrophilicity ... or to predict the chemical reactivity. These methods complement other approaches, such as the orbital analyses and provide a more complete picture of molecular interactions that would otherwise be difficult to obtain experimentally. The MoDerm 2023 school aims at introducing non-expert researchers to the main methods and tools of the electron density analysis. This school offers the opportunity to experience these specialized methods and tools from scratch. You will learn how they can be used to better understand molecular properties and chemical reactions. More advanced colleagues will also develop their expertise on these methods.

On behalf of the Organizing Committee

co-chairs
Julien Pilmé and Paul Fleurat-Lessard

ORGANIZING COMMITTEE

Julien Pilmé, chair, is an associate professor (Maître de Conférences) at Sorbonne University (Paris). He specializes in the development and implementation of quantum chemical topology approaches. He has expertise in their application to the chemical reactivity and for the analysis of relativistic effects in organic and organometallic chemistry. He is the developer of the TopChem2 software.

Paul Fleurat-Lessard, co-chair, is a professor at University of Bourgogne (Dijon). He specializes in the theoretical determination of organic and organometallic mechanisms and he has expertise in application of quantum chemical topology tools to the chemical reactivity. He is the developer of the Opt'n Path software designed to the reaction path construction.

Isabelle Fourré is an associate a professor (Maîtresse de Conférences) at Sorbonne University (Paris). Her research, in the field of theoretical astrochemistry, focuses on unravelling the reactivity of interstellar molecules in the gas phase using quantum chemistry. She also specializes in quantum chemical topology applied to the bonding analysis and to the chemical reactivity.

Franck Fuster is an associate professor (Maître de Conférences) at Sorbonne University (Paris). He specializes in the development, implementation of quantum chemical topology approaches and has developed an expertise in their application to the hydrogen bonding in (bio)organic chemistry. He is one of main developers of the TopMod package.

Frédéric Guégan is an associate professor (Maître de Conférences) at the university of Poitiers. He has developed an expertise in the modeling of chemical reactivity using the both explicit approaches (reaction paths) and implicit approaches (reactivity prediction with conceptual DFT and quantum chemical topology tools) .

Laurent Joubert is a professor at university Rouen Normandie. He specializes in the development, implementation, and application of quantum chemical topology appraoches and conceptual DFT descriptors. He is an official co-developer of the Amsterdam Density Functional (ADF) quantum chemistry package.

Vanessa Labet is an associate professor (Maîtresse de Conférences) at Sorbonne University (Paris). She has some expertise in the use of conceptual DFT descriptors and that of the non-covalent interactions index (NCI) for bonding analysis. Her research interest lies in the study of chemical reactivity under an external electric field.

Bruno Madebène is an associate professor (Maître de Conférences) at Sorbonne Université (Paris). He specializes in the calculations of extended systems and for their characterization using the quantum chemical topology. It has developed an expertise on the description of hydrogen bonding for its experimental characterisation.

Christophe Morell is a professor at university Claude Bernard of Lyon 1. His research interest mainly lies in the understanding of chemical reactivity, regio and stereo selectivity through quantum chemistry. He has developed several descriptors of the conceptual DFT (dual descriptor) designed to predict the chemical behavior of atomic sites within molecules.

Vincent Tognetti is an associate professor (Maître de Conférences) at university Rouen Normandie. He is a recognized expert in the development, implementation and application of quantum chemical topology approaches and conceptual DFT descriptors. He also specializes in the theoretical studies of UV-vis and NMR spectroscopies.

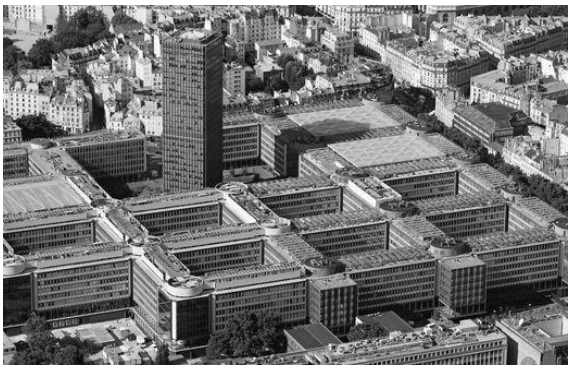
Emilie-Laure Zins is a professor at Sorbonne Université (Paris). She specializes in the quantum chemical topology applied to the chemical reactivity and to the analysis of the molecular electrostatic potential. She has developed an expertise on the description of the influence of the micro-hydration to the reactivity and its experimental characterization.

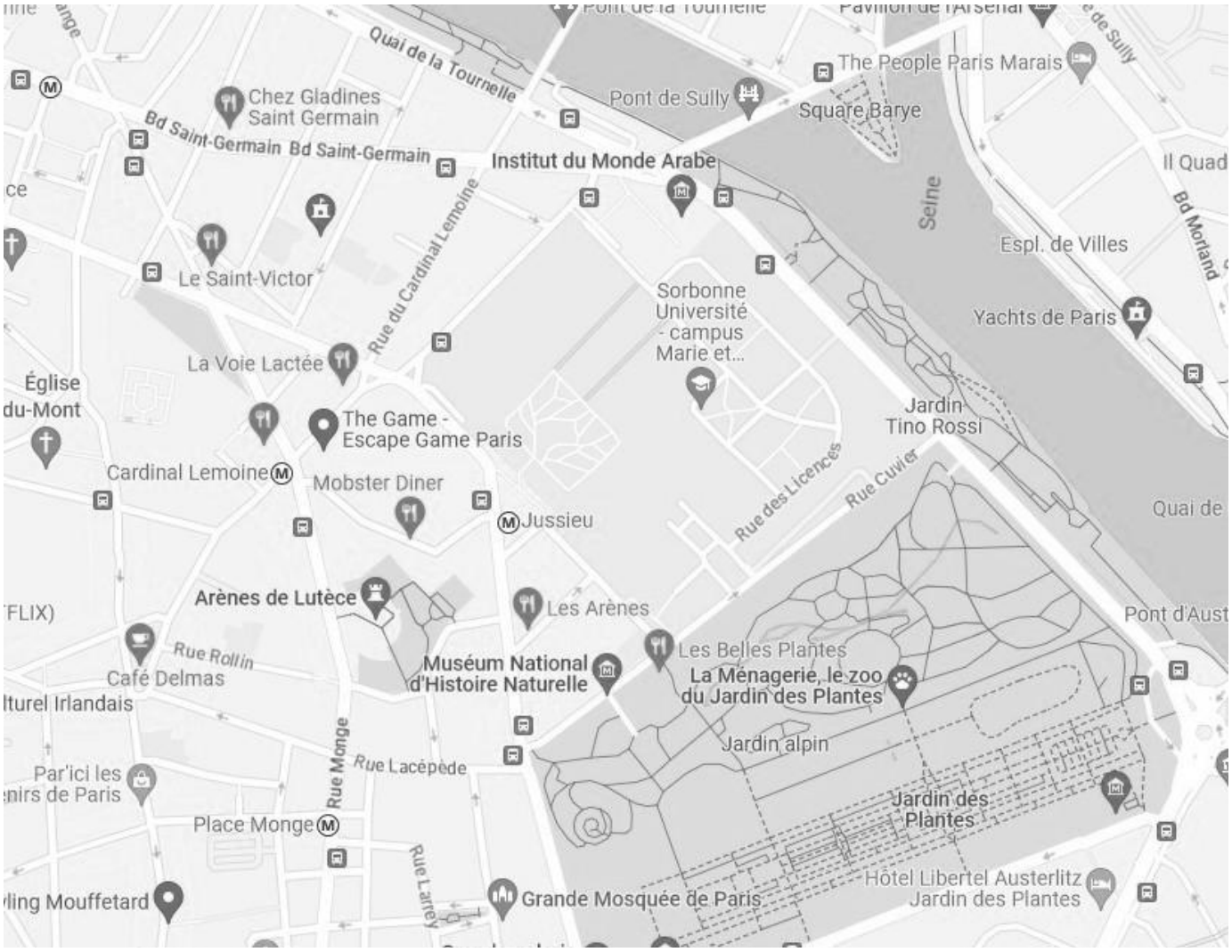
List of Participants MoDerm 2023

1	Arif	Muhammad Bilal	IMT MINES
2	Aroule	Olivier	Sorbonne université
3	Benchouk	Wafaa	Université de Tlemcem
4	Blanchet	Jérôme	ENSI Caen
5	Bonnefoy	Christelle	Université de Lyon
6	Carcabal	Pierre	Université Paris Sud
7	Carenco	Sophie	Sorbonne université
8	Cayla	Mattéo	Université de Bordeaux
9	Chataigner	Isabelle	Université de Rouen
10	Dupont	Nathalie	Université Sorbonne Paris Nord
11	Frison	Gilles	Sorbonne université
12	Gayraud	Oscar	Université de Poitiers
13	Giuliani	Alexandre	Synchrotron SOLEIL
14	Hédouin	Matthieu	Université de Rouen
15	Kenmogne Tchidjo	Joseline Flore	Université de Namur
16	Klein	Johanna	Université de Montpellier
17	Kossov	Arsene	Université Paris Sud
18	Longuet	Mélissa	Université de Poitiers
19	Malacea	Raluca	Université de Bourgogne
20	Memboeuf	Antony	Université de Brest
21	Mereau	Raphaël	Université de Bordeaux
22	Naghmouchi	Yathreb	Université de Namur
23	Nauton	Lionel	Université de Clermont
24	Penas	Francesc	Collège de France
25	Peter	Emmanuel	IMT MINES
26	Pouzens	Jean-Thomas	Universite de Bourgogne
27	Soulard	Pascale	Sorbonne université
28	Strekowski	Rafal	Aix-Marseille Université
29	Taamalli	Sonia	Université de Lille
30	Tasseau	Olivier	Université de Rennes
31	Vila Siles	Guillem	Donostia Physics Center

SCHOOL LOCATION

The school will take place on the Jussieu campus of the Faculty of Science and Engineering of Sorbonne University, 4 place Jussieu 75005 Paris (métro stop Jussieu line 7 or line 10) from Monday 4 September 2023 2 pm to Thursday 7 September 5 pm.





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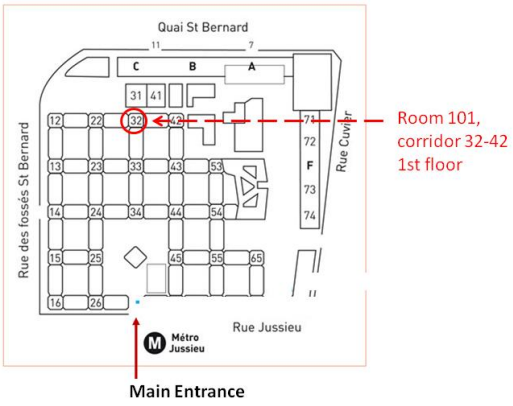
PROGRAM

Monday 4 sept.	Hands-on sessions	Tuesday 5 sept. T. 42-43, basement	Wednesday 6 sept. T. 42-43, basement	Thursday 7 sept. T. 42-43, basement
	Morning 9h30-12h30	QTAIM – IQA – REG	ELF, MESP & NCI	Conceptual DFT
	12h45	**Lunch** **Brasserie l'ardoise**	**Lunch** **Brasserie l'ardoise**	**Lunch** **Brasserie l'ardoise**
Tower 32, corridor 32-42, room 101 **13h45 Welcome at MoDerm 2023** **14h00-17h30 Theoretical aspects of the electron density analysis**	Afternoon 14h30-17h30	14h30-15h30 QTAIM – IQA - REG 16h -17h30 ELF, MESP &NCI	Conceptual DFT	hands on sessions and private discussions to research topic of participants.

Coffee Breaks :
- Morning : 11h
- Afternoon : 15h30



Monday 4 September

The first day will be devoted to the theoretical aspects of methods of analysis of interactions based on electron density. **The school will take place in the first floor of tower number 32, room 101, corridor 32-42.** After entering the campus look for tower number 32, then take the elevator, or the stairs to reach the first floor and the corridor 32-42.

13h45 ***Welcome at MoDerm 2023***

14h00 ***Introduction***

Chairman : Paul Fleurat-Lessard

14h10 Julien Pilmé : ***Introduction to Quantum Chemical Topology***

14h40 Laurent Joubert - Vincent Tognetti : ***QTAIM – IQA and REG approaches***

15h20 Julien Pilmé - Vanessa Labet : ***ELF - MESP and NCI approaches***

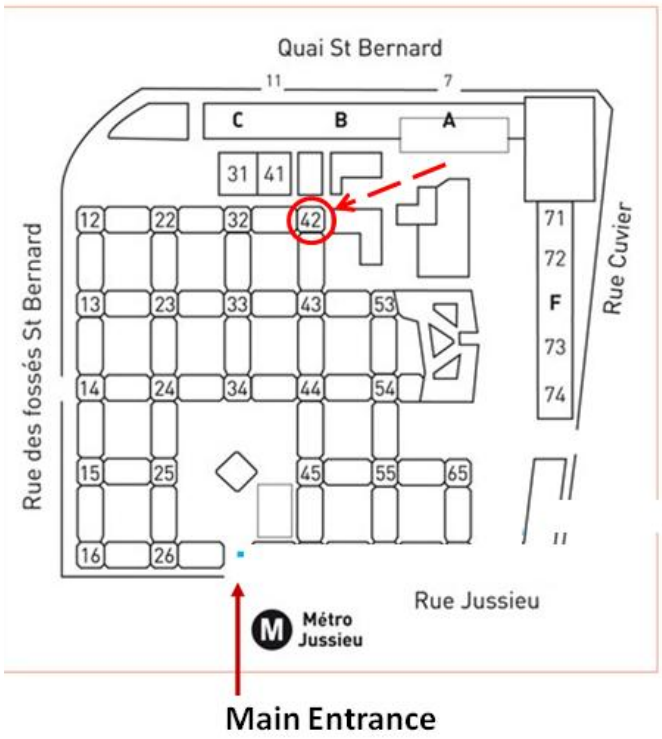
16h00 **Coffee break**

16h30-17h30 Fréderic Guegan – Christophe Morell – Vanessa Labet : ***Conceptual DFT***

From Tuesday 5 September to Thursday 7 September

The **hands-on computer sessions** will take place in two rooms located **in the basement of tower 42, corridor 42-43**. After entering the campus look for tower number 42, then take the stairs to reach the basement level.

ROOMS JACQUES LEVISALLES AND FICINI



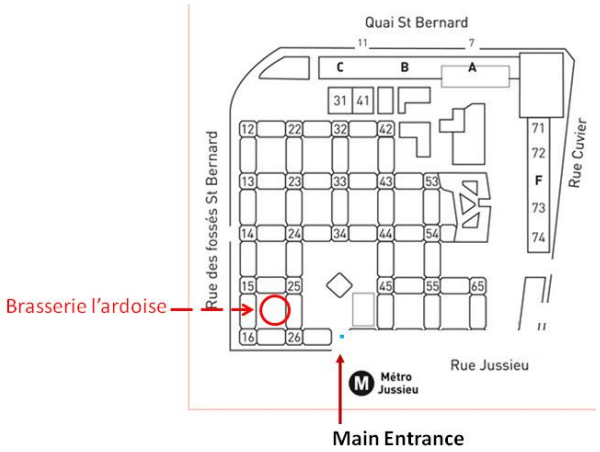
DOCUMENTS PDF AND FILES

https://moderm2023.sciencesconf.org/resource/page/id/9

PRACTICAL DETAILS

LUNCH 12h45 - Brasserie L'Ardoise - Tuesday 5, Wednesday 6 and Thursday 7 September.

The Brasserie L'Ardoise is located in the Jussieu campus :



FIAP ACCOMODATION AND MEALS

FIAP Jean Monet, 30 Rue Cabanis, 75014 Paris. https://www.fiap.paris/en/

Metro stop Glacière (line 6) near the Denfert-Rochereau station of the RER B (direct line with Roissy-Charles de Gaulle airport) and Orly-Bus.

Phone + 33 1 43 43 17 00

On September 4th, you can arrive at your convenience (luggage storage is available), but the rooms will **not** be available **before 2:30 PM**. When you arrive at the hotel reception, please provide your name and the name of the group (**MODERM** group). The FIAP staff will assign you a room based on your reservation (single or shared).

Room Check in : Monday 4 september, 2:30 pm
Room Check out: Thursday 7 september 9:00 am.

Breakfast and Dinner (**only If you have booked a room at the FIAP**). We would like to remind you that **breakfasts and dinners** will be provided by the school for the duration of your stay. A self-service catering will be offered to you, in the Cocagne space which consists of a bar and a self-service open on a terrace furnished with tables, deckchairs and parasols.

- Breakfast : 6h45 am to 9h am
- Dinner: 6h30 pm to 8h30 pm

https://www.fiap.paris/fiap-jeune/restauration/