

# Winter School on Quantum Metal-Organic Frameworks

Abstract Booklet

February 24-28, 2025



**CHALMERS**  
UNIVERSITY OF TECHNOLOGY

# Scope of the Winter School

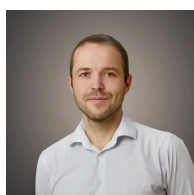
This one-week winter school focuses on metal-organic frameworks (MOFs) as quantum materials. The event builds a bridge between chemistry and condensed matter physics. The program is designed for PhD students, advanced Master's students, and PostDocs. Participants will explore cutting-edge theoretical and experimental methods, gaining a comprehensive understanding of this emerging research area.

## Funding sources

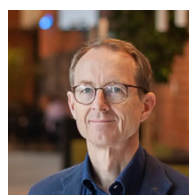
The winter school is made possible by generous support of the Chalmers Area of Advance Nano.



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# The Winter School - a 3 ECTS Course

Quantum materials host a variety of intriguing phenomena, based on many-body interactions or topology. While MOFs are often discussed in terms of their use in chemistry applications (catalysis, gas sorption, chemical sensing) their potential as quantum materials is only beginning to be explored. MOFs are network solids formed by metal ions or clusters linked by organic molecules, with tunable voids. Unlike conventional quantum materials, whose properties rely on charge, spin, orbital, and lattice, MOFs introduce unique degrees of freedom, including molecular buckling, torsion, rotation, and interpenetration, which can be tailored via supramolecular chemistry. To shape this promising research direction, the winter school aims to bring together experts from chemistry and condensed matter physics. This provides an excellent opportunity for building future research collaborations and disseminating knowledge to the next generation of experts.

## Course structure

The winter school is divided in on-site lectures (17 h), peer-discussions (3 h), a poster session (2 h) as well as one week of self-study (40 h) with selected reading material. The course assessment consists of a contribution to the poster session and a summary of a topic based on the selected reading materials (approximately two pages).

The expected learning outcomes are a basic familiarity with the following topics:

- Metal-organic frameworks
- Quantum materials
- 2D covalent frameworks and MOFtronics
- Topological electrons in MOFs
- Rotational dynamics and dynamic crystalline materials
- Emergence in MOFs

## Selected reading material

The self-study is based on the following reading material, complementary to the lectures provided.

- Z. Huang and R.M. Geilhufe: *Quantum Metal-Organic Frameworks* Small Sci. **4** 2400161
- W. Jiang, X. Ni and F. Liu: *Exotic Topological Bands and Quantum States in Metal-Organic and Covalent-Organic Frameworks* Acc. Chem. Res. **54** 416 (2021)
- A. Gonzalez-Nelson, F.X. Coudert and M.A. van der Veen: *Rotational Dynamics of Linkers in Metal-Organic Frameworks* Nanomaterials **2019** 9 330
- D. Kumar et al.: *Manifestation of Strongly Correlated Electrons in a 2D Kagome Metal-Organic Framework* Adv. Funct. Mater. **31** 2106474 (2021)
- L. Öhrström and F.M. Amombo Noa: *Metal-Organic Frameworks in Perspective* Chapter 1 in *Metal-Organic Frameworks* American Chemical Society (2020)
- T. Takenaka et al.: *Strongly Correlated Superconductivity in a Copper-Based Metal-Organic Framework with a Perfect Kagome Lattice* Sci. Adv. **7** eabf3996 (2021)
- C.G. Gruber et al.: *Early Stages of Covalent Organic Framework Formation Imaged in Operando* Nat. **630** 872 (2024)

## Lecturers

**Françoise M. Amombo Noa** is assistant professor at the University of Douala in Cameroon and guest researcher at the Department of Chemistry and Chemical Engineering at Chalmers University of Technology. She is currently working on synthesis and characterisation of metal-organic frameworks, covalent-organic frameworks and crystal engineering with emphasis on host-guest aspects and environmental applications. She is also specialised in structure determination by single crystal diffraction and is assisting Chalmers Materials Analysis Laboratory in this capacity.

**Feng Liu** is distinguished professor at the Department of Materials Science and Engineering at the University of Utah. His research focuses on material modeling and simulation from atomic to mesoscopic scales. His research group develops and applies both first-principles computational methods and phenomenological theoretical models to study a wide spectrum of material properties in various materials systems, such as topological materials, graphene, surfaces and interfaces and nanostructured materials.

**Monique A. van der Veen** is associate professor in the Department of Chemical Engineering at Delft University of Technology. Her research group investigates structure-property relationships of nanoporous materials, such as metal-organic frameworks, for applications in photo- and heterogeneous catalysis and electronics. An important part of her research is the use of advanced optical spectroscopy to gain detailed insight in the structure and function of nanoporous materials.

**Agustin Schiffrin** is associate professor at the School of Physics and Astronomy at Monash University in Melbourne. His research interests lie within the fields of experimental condensed matter physics, advanced materials, nanoscience and ultrafast photonics. His research deals with the synthesis of functional low-dimensional nanomaterials, characterised by low-temperature scanning probe techniques, x-ray absorption and photoelectron spectroscopies, and ultrafast time-resolved spectroscopies.

**Dana D. Medina** is researcher in the Department of Chemistry at Ludwig-Maximilians University Munich, where she leads a young research group and pursues her habilitation. Her research is focused on the design and synthesis of functional porous crystalline frameworks, particularly 2D layered structures. Large part of the research is dedicated to the development of novel on-surface deposition techniques with the goal of bringing periodic porous materials towards thin film applications in electronics, sensing and sieving.

**Nico Hahn** is researcher at the Department of Physics at Chalmers University of Technology. In his research he explores exactly solvable models for unconventional superconductivity in metal-organic frameworks.

# Location

The lectures will take place in the PJ lecture hall on Johanneberg Campus. The closest entrance is marked with the red arrow on the map below.



The location of the poster session is Scania hall shown on the map below.



An interactive version of this map can be found online under this link. Alternatively, you can download Find Your Way on Campus app on [App Store](#) or [GooglePlay](#).

## Schedule

### Monday, Feb 24th

09:30 - 10:30	Matthias Geilhufe - Introduction
10:30 - 11:00	Coffee break
11:00 - 12:00	Françoise Noa and Lars Öhrström - <i>Reticular Chemistry Synthesis: How to Make Metal-Organic Frameworks and Characterise Them</i>
12:00 - 13:30	Lunch break
13:30 - 14:30	Nico Hahn - <i>Quantum Materials and Emergent Phenomena</i>
14:30 - 15:00	Coffee break
15:00 - 16:00	Françoise Noa - <i>Reticular Chemistry Synthesis: How to Make Metal-Organic Frameworks and Characterise Them</i>
16:00 - 17:30	Welcome reception

### Tuesday, Feb 25th

09:30 - 10:30	Monique van der Veen - <i>Metal-Organic Frameworks: a Dynamic Playground</i>
10:30 - 11:00	Coffee break
11:00 - 12:00	Nico Hahn - <i>Quantum Materials and Emergent Phenomena</i>
12:00 - 13:30	Lunch break
13:30 - 14:30	Monique van der Veen - <i>Metal-Organic Frameworks: a Dynamic Playground</i>
14:30 - 15:00	Group photo and coffee break
15:00 - 16:00	Dana Medina - <i>Molecular Frameworks – Synthesis, Properties and Function</i>
16:00 - 16:15	Break
16:15 - 17:15	Literature seminar and discussion in parallel sessions
18:00 - 20:00	Speakers' Dinner

## Wednesday, Feb 26th

09:30 - 10:30	Dana Medina - <i>Molecular Frameworks – Synthesis, Properties and Function</i>
10:30 - 11:00	Coffee break
11:00 - 12:00	Feng Liu - <i>Topological Electronic States in MOFs</i>
12:00 - 13:30	Lunch break
13:30 - 14:30	Dana Medina - <i>Molecular Frameworks – Synthesis, Properties and Function</i>
14:30 - 15:00	Coffee break
15:00 - 16:00	Agustin Schiffrin - <i>Controllable Electronic Quantum Phases in 2D Metal-Organic Materials</i>
16:00 - 16:15	Break
16:15 - 17:15	Literature seminar and discussion in parallel sessions
18:00 - 20:00	Poster session

## Thursday, Feb 27th

09:30 - 10:30	Agustin Schiffrin - <i>Controllable Electronic Quantum Phases in 2D Metal-Organic Materials</i>
10:30 - 11:00	Coffee break
11:00 - 12:00	Françoise Noa - <i>Reticular Chemistry Synthesis: How to Make Metal-Organic Frameworks and Characterise Them</i>
12:00 - 13:30	Lunch break
13:30 - 14:30	Feng Liu - <i>Topological Electronic States in MOFs</i>

## Friday, Feb 28th

09:30 - 10:30	Nico Hahn - <i>Quantum Materials and Emergent Phenomena</i>
10:30 - 11:00	Coffee break
11:00 - 12:00	Feng Liu - <i>Topological Electronic States in MOFs</i>
12:00 - 13:30	Lunch break
13:30 - 14:30	Agustin Schiffrin - <i>Controllable Electronic Quantum Phases in 2D Metal-Organic Materials</i>
14:30 - 15:00	Coffee break
15:00 - 16:00	Literature seminar and discussion in parallel sessions

# Lecture Abstracts

## Reticular Chemistry Synthesis: How to Make Metal-Organic Frameworks and Characterise Them

Françoise M. Amombo Noa - University of Douala  
Lars Öhrström - Chalmers University of Technology

These three lectures will cover the basics of MOF chemistry in a way accessible to the nonspecialist scientist.

MOFs are known as coordination polymers and are materials of one-, two-, or three-dimensional networks formed by metal ions or clusters and bridging or multidentate organic linkers through coordination bonds [1].

We call this chemistry, Reticular Chemistry (from the Latin reticulum, meaning net), and the approach for the synthesis of reticulated materials such as metal-organic frameworks (MOFs), involves the conceptual formation of secondary building units (SBUs), usually both metal-SBUs and organic-SBUs [2].

There are approximately 100000 MOFs structures in the Cambridge Structural Database, synthesized via different methods. The general MOFs synthesis methods we are going to cover are classical solution chemistry, conventional solvothermal or hydrothermal synthesis, electrochemical synthesis, microwave, sonochemistry, mechanochemistry and more [3].

The basic characterizations of MOF materials are usually carried out by X-ray techniques, microscopy techniques and gas sorption. This will be covered in the final lecture.

### Literature:

- [1] Y. R. Lee, J. Kim and W. S. Ahn: *Synthesis of Metal-Organic Frameworks: A Mini Review* Korean J. Chem. Eng. **30** 1667 (2013)
- [2] O. M. Yaghi, M. J. Kalmutzki and C. S. Diercks: *Introduction to Reticular Chemistry - Metal-Organic Frameworks and Covalent Organic Frameworks* Wiley-VCH: Weinheim (2019)
- [3] L. Öhrström and F.M. Amombo Noa: *Metal-Organic Frameworks* American Chemical Society (2020)

# Topological Electronic States in MOFs

Feng Liu - University of Utah

In this three-lecture series, I will review and discuss important progresses made in the last decade in furthering our fundamental understanding of topological electronic states in organic frameworks, focusing on metalorganic frameworks (MOFs).

In lecture 1, I will first introduce the concept of topological insulators within the context of transport properties of solid-state materials [1]. I will then review and discuss the two-dimensional (2D) organic topological insulators (TIs) in MOFs, to recap the rapid developments of the fields of TIs in recent years. Especially, I will present studies of 2D TIs in MOFs, based on first-principles calculations and tight-binding model analyses, which are designed by assembling molecular building blocks of organometallic compounds with strong spin-orbit coupling into a hexagonal and/or Kagome lattices, including anomalous quantum Hall effect in magnetic TI MOFs.

In lecture 2, I will discuss lattice and orbital design of topological bands in organic frameworks [2], including MOFs and covalent organic frameworks (COFs), focusing especially on recent studies of molecular orbital design of Dirac and flat bands (FBs) in organic frameworks. I will outline a design principle based on the fundamental relationships between the electronic band structure, lattice symmetry, and characteristics of the frontier molecular orbitals of the building units. I will also discuss briefly the most recent experimental observation of topological FB in a H-bond organic frameworks (HOFs), enabled by growth of a self-assembled monolayer of 1,3,5-tris(4-hydroxyphenyl) benzene (THPB) on Au(111) substrate, a microsheet with high uniformity and long-range order.

In lecture 3, I will first introduce generally exotic quantum states associated with topological electronic states, potentially to be realized in organic frameworks. I will then present a detailed study of excitonic Bose-Einstein Condensation (BEC) in a quantum semiconductor consisting of flat valence and conduction bands of opposite chirality (so-called yin-yang FBs), as hosted in a diatomic Kagome lattice exemplified in superatomic graphene [3]. I will show that excitons can even have a negative formation energy in this organic framework, indicative of a triplet excitonic insulator state, based on DFT-GW and BSE calculations of a single exciton formation. I will also show directly spontaneous BEC of triplet excitons, based on analyses of multi-exciton formation energies and wave functions, using exact diagonalization method to solve an extended Hubbard lattice model of yin-yang FBs.

## Literature:

- [1] F. Liu: *Two-Dimensional Topological Insulators: Past, Present and Future* Coshare Science **01** 03 (2023)
- [2] W. Jiang, X. Ni and F. Liu: *Exotic Topological Bands and Quantum States in Metal-Organic and Covalent-Organic Frameworks* Acc. Chem. Res. **54** 416 (2021)
- [3] G. Sethi, M. Cuma and F. Liu: *Excitonic Condensate in Flat Valence and Conduction Bands of Opposite Chirality* Phys. Rev. Lett. **130** 186401 (2023)

# Metal-Organic Frameworks: a Dynamic Playground

Monique A. van der Veen - Delft University of Technology

Metal-organic frameworks are 3-D crystalline nanoporous materials build as frameworks from metal ions or inorganic clusters connected via organic linkers. They have been explored for a wide range of applications including adsorptive separations, sensing, catalysis, water harvesting, and so forth.

MOF structures are literally dynamic. Rotational dynamics of linkers and guest-induced deformations are very prevalent, and impact their behaviour in gas sorption, sensing and as stimuli-responsive materials. In rotor-MOFs ultrafast rotation can be engineering by decreasing the rotation energy barrier via molecular design. Yet, MOFs have, in fact, the potential of displaying much more intricate dynamics, similar to other dynamic materials containing closely interacting molecules, such as crowded movement of proteins in lipid bilayers, or concerted molecular motion in liquid crystals. MOFs in fact provide an exceptional playing ground, as they are offer a regular arrangement of rotors with defined intermolecular distances that can be tuned through the choice of building blocks. This means that the free pore space and inter-rotor distance can be tuned to a desired level of “crowdedness” of the achieve correlate linker motion. This will be the first lecture topic.

Similarly, for light-induced applications, the dynamics of the photo-excited charges are vital to the final performance in light-induced applications such as photocatalysis. While solar fuel production rates by MOFs are regularly reported, far less effort is invested in unravelling the pathway and dynamics of the photo-excited charges. As such my talk focusses on probing the ultrafast photodynamics of MOFs to enable the formulation of selection guidelines for photocatalytic MOFs. This will be the second lecture topic.

## Literature:

- J. G. Santaclara, F. Kapteijn, J. Gascon and M.A. van der Veen: *Understanding Metal–Organic Frameworks for Photocatalytic Solar Fuel Production* CrystEngComm **19** 4118 (2017)
- A. Gonzalez-Nelson, F.X. Coudert and M.A. van der Veen: *Rotational Dynamics of Linkers in Metal–Organic Frameworks* Nanomaterials **2019** 9 330

# Controllable Electronic Quantum Phases in 2D Metal-Organic Materials

Agustin Schiffrin - Monash University

Strong electron-electron Coulomb interactions in materials can lead to a vast range of exotic many-body quantum phenomena, including Mott metal-insulator transitions, correlation-induced magnetism, quantum spin liquids, and even unconventional superconductivity. Such many-body properties, resulting from correlations between electrons, depend strongly on the occupancy of the material's electronic states, and can hence be controlled via the material's chemical potential (e.g., via chemical doping, or electrostatically via the application of a gate electric field).

Two-dimensional (2D) materials with a frustrated (e.g., kagome, Lieb) crystal structure can host strongly localised electronic states and flat electronic bands, resulting from destructive interference between electronic wavefunctions. These flat bands enhance electron-electron interactions. As such, atomically thin 2D materials provide a useful platform for realising and exploring controllable correlated-electron quantum phases.

In particular, single-layer 2D covalent organic (COFs) and metal-organic (MOFs) frameworks – in which organic molecules act as building blocks – hold promise as functional electronic materials, given their versatile atomic-scale morphologies (and resulting electronic properties) that can be achieved via supramolecular self-assembly and metal-ligand coordination. Yet, correlated-electron phases in 2D COFs and MOFs with frustrated crystal structures remain relatively unexplored.

Here, I will talk about the electronic properties of single-layer 2D MOFs with a kagome crystal structure. As an example, I will focus on a specific 2D MOF consisting of flat aromatic molecules (9,10-dicyanoanthracene; DCA) arranged in a kagome structure via coordination with copper (Cu) atoms. When adsorbed on a weakly interacting metal surface – such as the (111) surface of silver – this 2D kagome MOF hosts local magnetic moments which, as shown by density functional theory and mean-field Hubbard modelling, are the consequence of strong electron-electron Coulomb interactions given by the kagome geometry [1,2]. On an atomically thin insulator – such as monolayer hexagonal boron nitride (hBN) on the (111) surface of copper (Cu) – the same 2D kagome MOF exhibits a 200 meV electronic energy gap which is consistent with dynamical mean-field theory predictions of a Mott insulating phase [3]. Relying both on the local work function variations of the hBN/Cu(111) substrate and on the electric field applied by the tip of a scanning probe microscope, we are able to locally tune the electron population of the kagome bands and to induce Mott metal-insulator transitions in this MOF on hBN/Cu(111). I will conclude by discussing prospects of electrostatically controlled correlated-electron phases in 2D MOFs on gateable 2D material heterostructures. Our findings pave the way for nanoelectronics and spintronics technologies based on 2D MOFs and on electrostatic control of many-body quantum phases therein.

## Literature:

- [1] D. Kumar et al.: *Manifestation of Strongly Correlated Electrons in a 2D Kagome Metal–Organic Framework* Adv. Funct. Mater. **31** 2106474 (2021)

- [2] B. Field, A. Schiffrin and N. V. Medhekar: *Correlation-Induced Magnetism in Substrate-Supported 2D Metal-Organic Frameworks* npj Comput. Mater. **8** 227 (2022)
- [3] B. Lowe et al.: *Local Gate Control of Mott Metal-Insulator Transition in a 2D Metal-Organic Framework* Nat. Commun. **15** 3559 (2024)

# Molecular Frameworks – Synthesis, Properties and Function

Dana D. Medina - Ludwig-Maximilians-University Munich

Crystalline and porous molecular framework materials with specific encoded properties hold promise as a novel, highly tunable, functional platform [1]. Through the concepts of reticular chemistry, numerous two- and three-dimensional molecular frameworks with diverse structural, optical, and electrical properties are in reach. However, the way 2D covalent organic frameworks (COFs) form in solution, in the absence of an obvious templating interface, remains a subject of scientific debate. On-surface deposition of molecular framework coatings is crucial for their utilization as active layers in advanced device-based applications, including separation, sensing and optoelectronics. In addition to the variable backbone properties, gaining control over the molecular framework film morphology is of critical importance for achieving the intended functionality [2].

In the presentation, I will first provide an overview of the synthesis of 2D molecular frameworks, focusing on the design strategies used to achieve highly ordered structures. Subsequently, the leading proposed COF growth mechanisms and new insights into COF formation will be discussed [3,4]. Following this, I will present the on-surface synthesis of COFs as films and deposits, with a particular emphasis on in-situ and vapor-assisted conversion approaches that enable the formation of crystalline COF films, thereby enhancing their utilization [2,5,6].

## Literature:

- [1] A. Mähringer and D. D. Medina: *Taking Stock of Stacking* Nat. Chem. **12** 985 (2020)
- [2] D.D. Medina et al.: *Photoactive and Conducting Covalent Organic Frameworks* Adv. Energy Mater. **2017** 1700387
- [3] A.M. Evans et al.: *Two-Dimensional Polymers and Polymerizations* Chem. Rev. **122** 442 (2022)
- [4] C.G. Gruber et al.: *Early Stages of Covalent Organic Framework Formation Imaged in Operando* Nat. **630** 872 (2024)
- [5] J.W. Colson et al.: *Oriented 2D Covalent Organic Framework Thin Films on Single-Layer Graphene* Science **332** 228 (2011)
- [6] D.D. Medina et al.: *Room Temperature Synthesis of Covalent–Organic Framework Films through Vapor-Assisted Conversion* J. Am. Chem. Soc. **137** 1016 (2014)

# Quantum Materials and Emergent Phenomena

Nico Hahn - Chalmers University of Technology

To start off the physics part of the winter school, I will introduce some concepts fundamental to later lectures on quantum effects in metal-organic frameworks (MOFs). The first key concept is the electronic band structure, which emerges due to the lattice periodicity of the MOF (or any other crystal) and serves as the foundation for our understanding of electronic properties in crystalline materials. A later series of lectures is concerned with topologically non-trivial electronic band structures. While topology may initially seem like a purely mathematical detail, it impacts the electronic structure at the boundary of the systems, resulting in the quantization of transport coefficients. Furthermore, I will briefly address the role of electron-electron interactions in materials. In weakly interacting systems, this effect can be absorbed into the effective mass of the electron and leads only to numerical corrections. In strongly interacting systems, however, new kinds of physics can emerge. A notable example is the Mott insulator: a material that is predicted to be conducting by the band structure, but is insulating instead.

The major part of my lectures focuses on the quantum phenomenon of superconductivity [1,2]. We begin with the earliest macroscopic theory of superconductivity. London theory provides a connection between the two universal macroscopic phenomena in superconductors: a vanishing resistivity and the expulsion of magnetic fields from the material (known as the Meißner-Ochsenfeld effect). In passing, we revisit concepts of electrodynamics necessary for the derivation of the theory. This is followed by a primer on the microscopic Bardeen-Cooper-Schrieffer (BCS) theory of conventional superconductors. Finally, we discuss aspects of superconductivity in the two-dimensional MOF Cu-BHT, the first MOF discovered to exhibit superconductivity [3].

## Literature:

- [1] J. F. Annett: *Superconductivity, Superfluids and Condensates* Oxford University Press (2004)
- [2] Richard Behiel: *Superconductivity and the Higgs Field* YouTube (2025)
- [3] T. Takenaka et al.: *Strongly Correlated Superconductivity in a Copper-Based Metal-Organic Framework with a Perfect Kagome Lattice* Sci. Adv. **7** eabf3996 (2021)