



UNIVERSITÀ DEGLI STUDI
DELL'INSUBRIA

“Materials Science for Catalysis, Adsorption and Separation”

Coordinator: Prof. Jenny G. Vitillo

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Keywords: porous materials, heterogeneous catalysis, metal–organic frameworks (MOFs), zeolites, metal nanoparticles, gas adsorption, gas separation, CO₂ capture, spectroscopic characterization, computational modeling.



Purpose: The facility is dedicated to the design, synthesis, characterization, and modeling of functional materials for applications in heterogeneous catalysis, gas adsorption and separation, and light harvesting. The main objective is the development of advanced materials and the molecular-level understanding of interactions between solid surfaces and guest molecules through the integration of experimental and computational approaches.

Examples of applications

- Catalysts based on metal–organic materials and metal nanoparticles for C–H bond activation and hydrogenation reactions.
- Porous materials for CO₂ and H₂ capture, storage, and separation, as well as for industrial gas separation.
- Investigation of dyes encapsulated in microporous materials for light harvesting, light upconversion, and photonics applications.
- Support for the development of materials for sustainable energy and environmental processes.

Location: Department of Science and High Technology, Via Valleggio 9, 22100 Como.

Organization:

The facility integrates experimental and theoretical expertise in materials science, combining chemical synthesis, structural and spectroscopic characterization, and advanced computational modeling. It serves as a reference center for the development and investigation of functional materials for catalytic, energy, and environmental applications.

The facility is organized into three sub-units:

- Sub-unit 1 – Synthesis and Design of Functional Materials
- Sub-unit 2 – Catalysis, Adsorption and Separation
- Sub-unit 3 – Advanced Characterization and Computational Modeling

Connections with the CRIETT Technological Platforms and the University Scientific Platforms:

The facility operates in collaboration with:

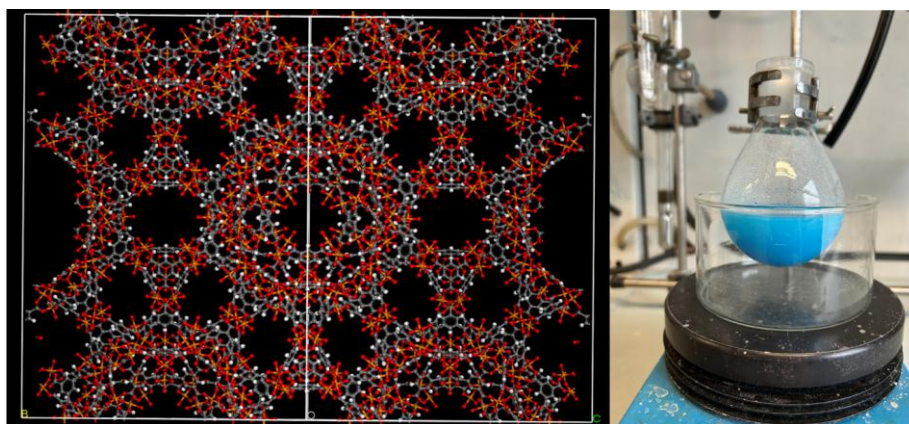
- Sustainability Platform, with reference to the objectives of (i) sustainability of industrial processes, (ii) reduction of environmental impact, (iii) capture and valorization of waste streams, and (iv) protection of natural resources.
- Technologies for Energy, Health and Environment Platform, in the framework of the development of materials, methods, and approaches for advanced energy and environmental applications.

Sub-unit “Synthesis and Design of Porous and Nanostructured Materials”

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Keywords: materials synthesis, metal–organic frameworks (MOFs), zeolites, metal nanoparticles, microporous materials, hydrothermal techniques, glove box.



Brief Description

The facility is dedicated to the synthesis and rational design of functional materials, with particular focus on microporous and nanostructured materials for applications in catalysis, adsorption, and separation. Activities include the synthesis of metal–organic frameworks (MOFs), zeolites, and hybrid materials, as well as the preparation of supported and unsupported metal nanoparticles.

The sub-unit has consolidated expertise in the handling of air- and moisture-sensitive compounds through the use of inert-atmosphere glove boxes, as well as in the application of hydrothermal techniques for the controlled synthesis of porous materials. The integrated approach enables modulation of the composition, structure, and surface properties of materials, optimizing their performance according to the targeted application.

Publications:

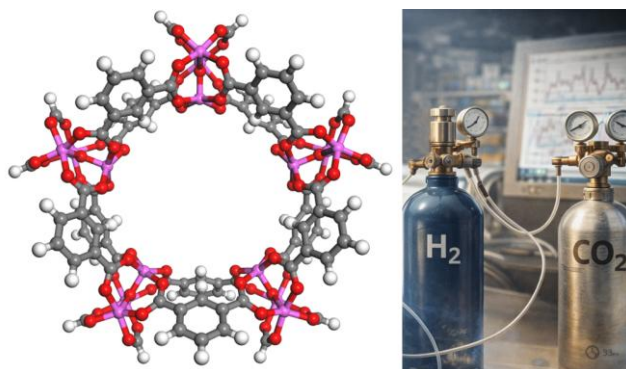
1. "Influence of First and Second Coordination Environment on Structural Fe(II) Sites in MIL-101 for C–H Bond Activation in Methane", J.G. Vitillo, C.C. Lu, C.J. Cramer, A. Bhan, L. Gagliardi, *ACS Catal.*, **11**, 579–589 (2021).
2. "Modeling Metal Influence on the Gate Opening in ZIF-8 Materials", J. G. Vitillo, L. Gagliardi, *Chem. Mater.* **33**, 4465–4473 (2021). [featured on the Front Cover]
3. "Experimental and computational characterization of phase transitions in CsB₃H₈", O. Zavorotynska, M. H. Sørby, J. G. Vitillo, S. Deledda, C. Frommen and B. C. Hauback, *Phys. Chem. Chem. Phys.*, **23**, 17836–17847 (2021).
4. "Water-Driven Structural Transformation in Cobalt Trimesate Metal-Organic Frameworks", J. Ethiraj, V. Surya, P. Selvam and J. G. Vitillo, *Energies*, **14**, 4751 (2021).
5. "Catalytic, Spectroscopic, and Theoretical Studies of Fe₄S₄-Based Coordination Polymers as Heterogenous Coupled Proton–Electron Transfer Mediators for Electrocatalysis", N. Jiang, A. Darù, Š. Kunstelj, J. G. Vitillo, M. E. Czaikowski, A. Filatov, A. Wuttig, L. Gagliardi, J. S. Anderson,* *J. Am. Chem. Soc.*, **146**, 12243–12252 (2024). DOI: <https://doi.org/10.1021/jacs.4c03726>
6. "Introducing Metal-Sulfur Active Sites in Metal-Organic Frameworks via Post-Synthetic Modification for Hydrogenation Catalysis", *Nature Chem.* (2025). DOI: <https://doi.org/10.1038/s41557-025-01876-y>

Sub-unit “Heterogeneous Catalysis and Adsorption/Separation”

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Keywords: heterogeneous catalysis, hydrogenation, C–H activation, gas adsorption, CO₂ capture, H₂ storage, adsorption volumetry.



Brief Description

The facility is dedicated to the investigation of the catalytic and adsorption properties of the materials developed within the facility, with particular focus on heterogeneous catalysis processes, CO₂ capture and separation, and gas storage. Activities include the use of MOF-based catalysts (particularly iron-based systems) for C–H bond activation and metal nanoparticles for hydrogenation reactions.

The sub-unit will employ adsorption volumetry techniques (instrument currently under acquisition) for the determination of specific surface area, pore size distribution, and adsorption capacity toward N₂, CO₂, and H₂. These measurements provide a quantitative assessment of material performance in energy and environmental applications, supporting the development of sustainable and highly efficient solutions.

Publications:

1. “Thermal Treatment Effect on CO and NO Adsorption on Fe(II) and Fe(III) Species in Fe₃O-Based MIL-Type Metal–Organic Frameworks: A Density Functional Theory Study”, Vitillo, J. G.; Gagliardi, L. *Inorg. Chem.* **60**, 11813–11824 (2021).
2. “Beyond Radical Rebound: Methane Oxidation to Methanol Catalyzed by Iron Species in Metal–Organic Framework Nodes”, M. C. Simons, S. D. Prinslow, M. Babucci, A. S. Hoffman, J. Hong, J. G. Vitillo, S. R. Bare, B. C. Gates, C. C. Lu, L. Gagliardi and A. Bhan, *J. Am. Chem. Soc.*, **143**, 12165–12174 (2021).
3. “The role of carbon capture, utilization and storage for economic pathways that limit global warming to below 1.5 °C”, J. G. Vitillo, M. D. Eisaman, E. S. P. Aradóttir, F. Passarini, T. Wang, S. W. Sheehan, *iScience*, **25**, 104237 (2022).
4. “Comparing the reaction profiles of single-iron catalytic sites in enzymes and in reticular frameworks for methane-to-methanol oxidation”, J. G. Vitillo,* C. C. Lu, A. Bhan, L. Gagliardi, *Cell Rep. Phys. Sci.* **4**, 101422 (2023).
5. “Mechanism of Benzene Hydroxylation on Tri-Iron Oxo-Centered Cluster-Based Metal–Organic Frameworks”, J. G. Vitillo*, M. Choudhary, M. C. Simons, L. Gagliardi and A. Bhan,* *J. Phys. Chem. C*, **127**, 23246–23257 (2023). DOI: 10.1021/acs.jpcc.3c06423
6. “Unraveling Transfer Hydrogenation Mechanisms by Ammonia Borane to Alkenes Over Self-Healing Copper Nanoparticles: the Complementary Role of N-H Bond, Surface, and Solvent”, A. Maspero, F. Bardelli, K. F. Konidaris, M. Uboldi, C. Lucarelli, N. Schiaroli and J. G. Vitillo*, *ACS Catal.*, **14**, 9594–9606 (2024). DOI: <https://doi.org/10.1021/acscatal.4c02556>
7. “Introduction to hybrid pores for CO₂ technologies”, P. Ágota Szilágyi, J. G. Vitillo, G. A. Craig, *Mater. Adv.*, **5**, 5336–5338 (2024). DOI: <https://doi.org/10.1039/D4MA90055C>

Sub-unit “Spectroscopic Characterization and Computational Modeling of Materials”

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Keywords: FTIR, UV–Vis, Raman, TGA, DSC, XRPD, DFT, TD-DFT, multireference methods, molecular modeling, machine learning, artificial intelligence.



Brief Description

The facility is dedicated to the structural, thermal, and spectroscopic characterization of materials and to the investigation of their interactions with guest molecules through the integration of experimental and computational approaches. Experimental activities include FTIR spectroscopy (both transmission and ATR modes) and UV–Vis spectroscopy in homogeneous and heterogeneous phases, thermal analyses (TGA and DSC), XRPD for quality control and structural stability assessment, as well as SEM for morphological analysis.

The sub-unit has a strong quantum-mechanical modeling component based on DFT, TD-DFT, and multideterminantal methods for the simulation of reaction profiles and the assignment of IR and Raman spectra of probe molecules (CO, H₂, CO₂, NO, etc.) interacting with solid surfaces, as well as UV–Vis spectra of optically active molecules for light harvesting and light upconversion applications. The integration of experimental data and simulations enables an in-depth understanding of the mechanisms underlying catalytic and adsorption processes. Artificial intelligence and machine learning methods are also employed for materials design.

Publications:

1. “Multireference methods are realistic and useful tools for modeling catalysis”, J. G. Vitillo, C. J. Cramer, L. Gagliardi, *Isr. J. Chem.*, **62**, e202100136 (2022).
2. “X-ray and synchrotron FTIR studies of partially decomposed magnesium borohydride”, R. Dahal, J. G. Vitillo, A. C. Åsland, C. Frommen, S. Deledda and O. Zavorotynska, *Energies*, **15**, 7998 (2022).
3. “Synthesis, Characterization, Fluorescence Properties, and DFT Modeling of Difluoroboron Biindole-diketonates”, A. Maspero, F. Vavassori, L. Nardo, G. Vesco, J. G. Vitillo,* and A. Penoni,* *Molecules*, **28**, 4688 (2023).
4. “Best practices for transition metal catalysts with density functional methods”, J. G. Vitillo,* *Chem Catal.*, **5**, 101427 (2025). DOI: <https://doi.org/10.1016/j.cheecat.2025.101427>
5. “Breaking the 1250 nm Barrier: A Computational Approach to Light Upconversion via Triplet-Triplet Annihilation in the Silica Telecom Band”, J. G. Vitillo, *ACS Applied Energy Mater.*, accepted (2026).

1) Synthesis and Design of Porous and Nanostructured Materials



Laboratory Glassware and Basic Instrumentation for Chemical Reactions

Laboratory glassware and instrumentation dedicated to the preparation of solutions and the execution of chemical reactions under controlled conditions, supporting the synthesis of porous and nanostructured materials.



LLG uniOVEN-110

StuLaboratory oven for the synthesis and thermal treatment of materials, equipped with accurate temperature control ($\pm 0.5\text{ }^{\circ}\text{C}$), essential to ensure reproducibility and control of crystallization processes.



Reactors for Solvothermal and Hydrothermal Synthesis

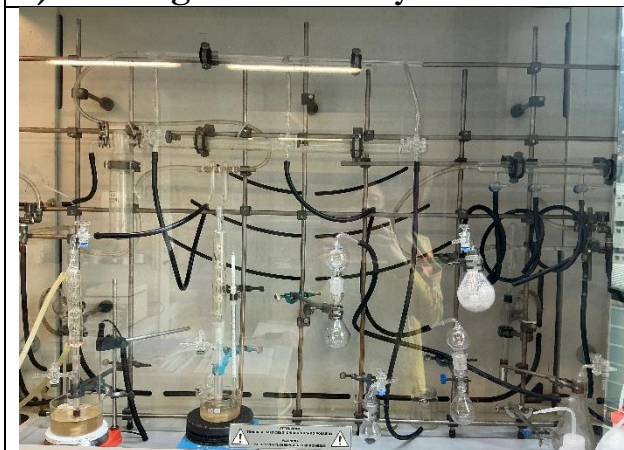
High-pressure Teflon-lined and stainless-steel reactors for the solvothermal and hydrothermal synthesis of microporous materials, enabling precise control of temperature, pressure, and reaction time.



MBRAUN Labstar Three-Glove Glove Box

Controlled-atmosphere (argon) glove box system for the handling and synthesis of air- and moisture-sensitive compounds, ensuring reproducible operating conditions and high purity of the obtained materials.

2) Heterogeneous Catalysis and Adsorption/Separation



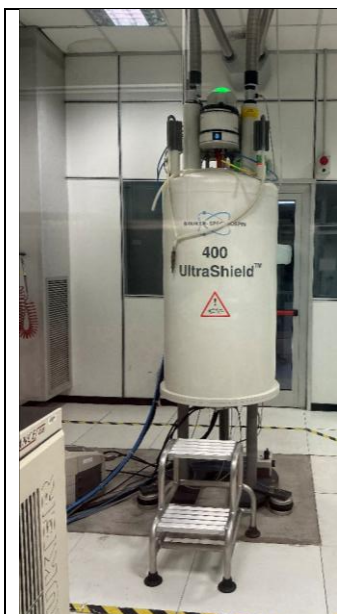
Schlenk line

Schlenk line for the handling and reaction of air- and moisture-sensitive compounds under inert atmosphere, used in the preparation and investigation of heterogeneous catalysts.



MBRAUN Labstar Three-Glove Glove Box

Controlled-atmosphere (argon) glove box system for the handling and synthesis of air- and moisture-sensitive compounds, ensuring reproducible operating conditions and high purity of the obtained materials.



NMR, TGA–DSC, SEM, XRD (currently under acquisition), volumetric adsorption analyzer (currently under acquisition), GC–MS. Further details are available on the CRIETT webpage.

<https://www.uninsubria.it/ricerca/strutture-la-ricerca/centri-speciali/centro-di-ricerca-e-trasferimento-tecnologico-criett-1>

3) Spectroscopic Characterization and Computational Modeling of Materials



Thermo Fisher Scientific Nicolet iS10 FTIR Spectrometer (DTGS Detector)

FTIR spectrometer operating in the 4000–650 cm^{-1} range, used for the investigation of molecular vibrations and interactions between probe molecules and solid surfaces, in both transmission and ATR modes.



Shimadzu UV-2600i UV-Vis Spectrophotometer

UV-Vis spectrophotometer for transmission and diffuse reflectance measurements in the 185–900 nm range, with 0.5 nm resolution, used for the analysis of the optical and electronic properties of materials.

NMR, TGA–DSC, SEM, XRD (currently under acquisition), see above.