2025 Syensqo chair in chemistry by the International Solvay Institutes

Professor Laura Gagliardi

University of Chicago, USA

Inaugural Lecture

Theory, Computation and Machine Intelligence for Reticular Chemistry

I will describe the synergies of theory, computation, and machine intelligence to expedite the discovery of innovative reticular materials, with a particular focus on their application in catalysis and water harvesting.

I will first discuss our current endeavors in understanding and optimizing the water-harvesting potential of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) by the elucidation of the water-filling mechanism. [1], [2].

I will then present a comprehensive computational and data-driven investigation, complemented by experimental work, focusing on sulfur-based MOFs for electrocatalytic transformations relevant to hydrogenation and CO2 reduction.[3] The computational insights have played a pivotal role in guiding the synthesis of novel MOFs. Initiating our study with previously reported Fe4S4 chain coordination polymers, we systematically explore the influence of alternative linkers and counter-cations on the material's structure. This investigation aims to tailor these materials into porous 2D or 3D frameworks. Notably, our efforts have resulted in the development of a computational workflow for MOF and COF structure prediction.[4]

[1] N. Hanikel, D. Kurandina, S. Chheda, Z. Zheng, Z. Rong, S. E. Neumann, J. Sauer, J. I. Siepmann, L. Gagliardi, and O. M. Yaghi, MOF Linker Extension Strategy for Enhanced Atmospheric Water Harvesting, ACS Central Science., 2023, 9, 551–557, DOI: 10.1021/acscentsci.3c00018.
[2] D. Kurandina, B. Huang, W. Xu, N. Hanikel, A. Darù, G.D. Stroscio, K. Wang, L. Gagliardi,
F.D. Toste, O.M. Yaghi, A Porous Crystalline Nitrone-Linked Covalent Organic Framework A. C. Int. Ed. 2023, 62, e202307674 DOI: 10.1002/anie.202307674
[3] N. Jiang, A. Darù, Š. Kunstelj, J. G. Vitillo, M.E. Czaikowski, A. Wuttig, L. Gagliardi, J.S. Anderson. Catalytic, Spectroscopic, and Theoretical Studies of Fe4S4-Based Coordination Polymers as Heterogenous CPET Mediators for Electrocatalysis J. Am. Chem. Soc., 2024, 146, 12243–12252. DOI: 10.1021/jacs.4c03726
[4] A. Darù, J. Anderson, D. Proserpio, and L. Gagliardi, Symmetry is the Key to the Design of Reticular Frameworks, ChemRxiv, 2024. DOI: 10.26434/chemrxiv-2024-37wks

TUESDAY 28 JANUARY 2025 AT 4:00 PM

COFFEE AND TEA WILL BE SERVED AT 3:45 P.M AND DRINKS AT 5:00 P.M. IN FRONT OF THE SOLVAY ROOM

The inaugural lecture will be followed by three other lectures on:
Tuesday 18 February - Tuesday 2 September - Tuesday 28 October

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Quartier Jaune - Building N.O. - 5th Floor - Solvay Room