The Chemist's Interactions

Seminars @ the Chemistry Department

Room G14 h 11.00

Monday, 23rd June 2025

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Advancing Reticular Chemistry with Generative AI

In this talk, I will introduce recent developments in leveraging generative AI to accelerate the discovery of new materials in reticular chemistry, with a focus on applications such as atmospheric water harvesting [1]. Generative AI — particularly large language models (LLMs) capable of processing and generating scientific text — is fundamentally transforming the research landscape [2]. Over the past eighteen months, we have developed a series of tools that enable the deployment of LLMs across various stages of the experimental synthesis workflow. These tools include purpose-built AI agents tailored to address domain-specific challenges in reticular chemistry, such as extraction of synthesis conditions, literature summarization, and candidate material screening [3]. I will also present our recent work on RetChemQA [4], a dataset comprising 95,000 question–answer pairs curated from the scientific literature. This dataset is designed to support the fine-tuning and evaluation of LLMs on chemistry-specific tasks and underscores the central role of data quality in AI development — the performance of any model is ultimately constrained by the quality of its training data. I will conclude with a discussion on emerging directions for generative AI in materials science, and how these tools may accelerate the design and discovery of reticular materials.

(1) *J. Am. Chem. Soc.* **2023**, *145* (51), 28284.
(2) *Nat. Rev. Mat.* **2025**. DOI: 10.1038/s41578-025-00772-8.
(3) *ACS Cent. Sci.* **2023**, *9* (11), 2161.
(4) *J. Chem. Theory. Comput.* **2024**, *20* (20), 9128.

The event will be streamed on MS Teams for external participants!

For registrations: seminari.dipchi@unimi.it

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