



ICSC Innovation and Community Day

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**DAMA - Tecnopolo Data Manifattura
Emilia-Romagna (Bologna)**

HPCvsCO2 Machine Learning and Quantum Computing for the design of high- performance materials for CO2 capture and conversion

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 **ICSC Innovation and Community Day**

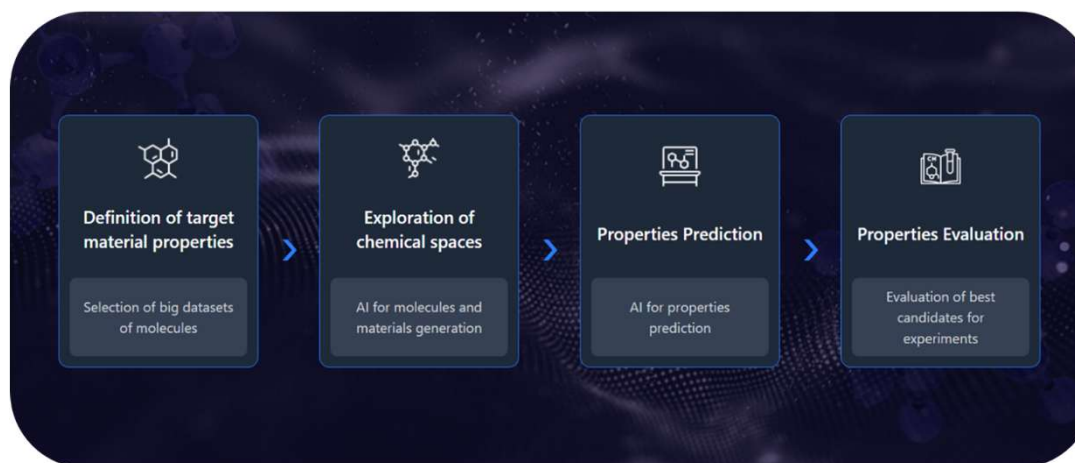
Introduction

The **HPCvsCO₂** project represents a comprehensive effort to **boost** molecular **catalyst discovery for CO₂ capture and conversion**.

Catalysts development through classical computational chemistry is resource-intensive and limited in exploration of chemical space.

The research integrates **High-Performance Computing (HPC)**, **Machine Learning (ML)**, and **Generative Artificial Intelligence (GenAI)** to accelerate the identification of promising catalytic systems. **Quantum Computing** is explored to further enhance the discovery process.

The focus centers on **metal-salen complexes** as catalysts to convert CO₂ into reusable products. The catalyst could be used again for new catalytic cycles.



Partners and collaboration model



Core Expertise

- Advanced Artificial Intelligence & Data Informatics.
- Machine Learning and Deep Learning architectures.
- Quantum Computing integration.

Technical Capabilities

- Data Processing & Analytics: Large-scale molecular dataset processing, feature extraction, and statistical analysis.
- Predictive Modeling: Development of ML models for molecular property prediction.
- Generative AI Systems: Integration of AI algorithms for generation of novel molecular structure.
- Full-Stack Development: End-to-end software solutions, and user interface development.



Core Expertise

- Advanced Chemical Sciences & Molecular Theory.
- Computational Chemistry methodologies.
- Laboratory-scale synthesis and characterization.

Technical Capabilities

- Chemistry Software & Computation: Molecular modeling, quantum chemistry calculations and simulation tools.
- Output Validation & Assessment: Scientific evaluation of AI-generated molecular candidates and feasibility analysis.
- Laboratory Integration: Target-oriented experimental design and synthesis pathway development.
- Quality Assurance: Chemical accuracy verification and practical implementation guidance.

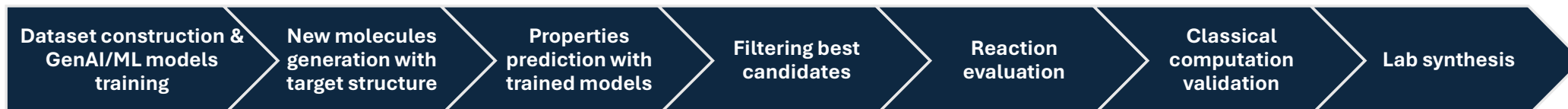
Computational Workflow

Traditional Workflow



In the traditional computational chemistry context, the real bottleneck is to run classical computation on all the new designed molecules: these calculations are computationally expensive so the try-and-repeat approach in designing new molecules is very time-consuming (years).

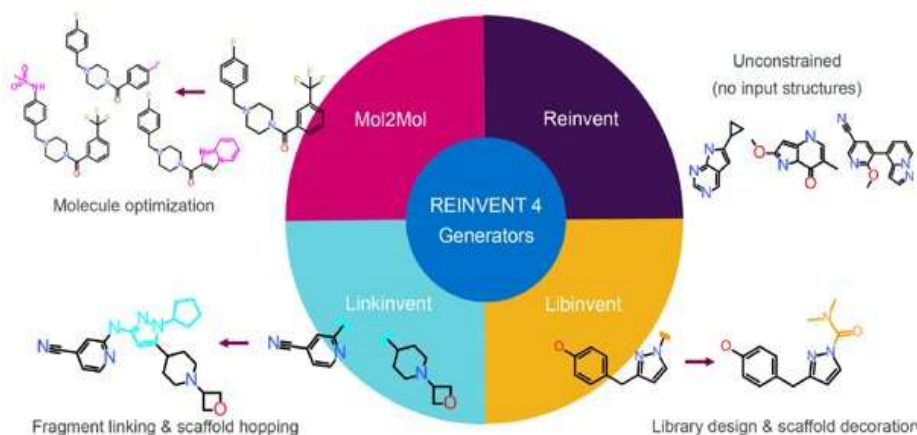
Materials Informatics Workflow



HPCvsCO₂ proposes a data-driven approach in the Material Informatics paradigm where GenAI models generate new molecular candidates and Machine Learning models predict their properties rapidly. This enables efficient pre-screening and filtering, reserving expensive computational chemistry calculations only for the most promising candidates, reducing computational costs while maintaining discovery effectiveness.

ML and AI models

State-of-the-art AI techniques are fine-tuned, covering both data-driven solutions for novel molecule generation (GenAI Reinvent 4 model) and predictive models for molecular property prediction (UniMol and UMA by Meta ML models).



Training dataset: ~100,000 transition metal complexes (TMQM public dataset) + 30,000 novel metal-salen complexes.

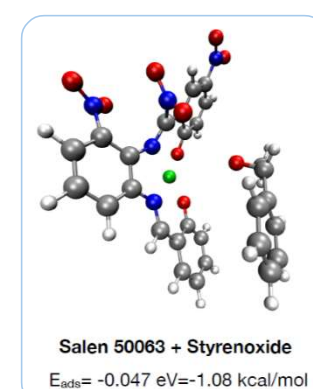
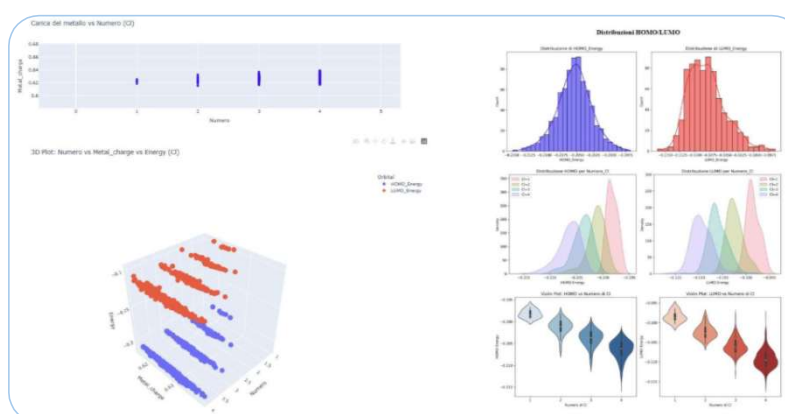
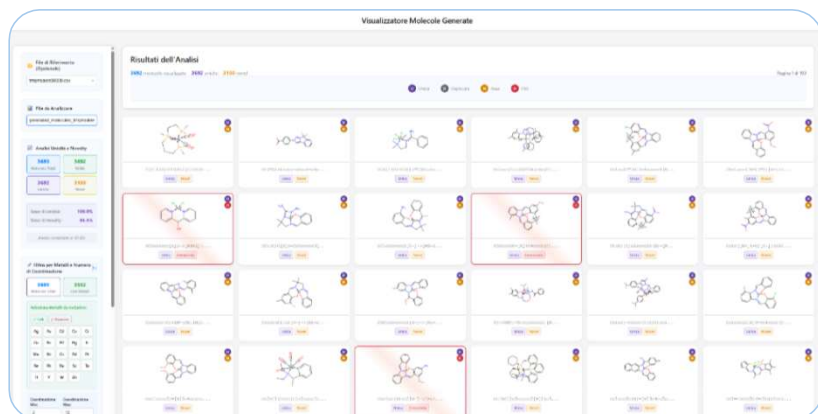
Results

Expert-based filtering and validation criteria were developed by combining domain expertise from catalyst specialists with comprehensive literature analysis.

The evaluated properties span geometric, electronic and energetic descriptors, with selection criteria targeting catalysts that are energetically favorable for CO₂.

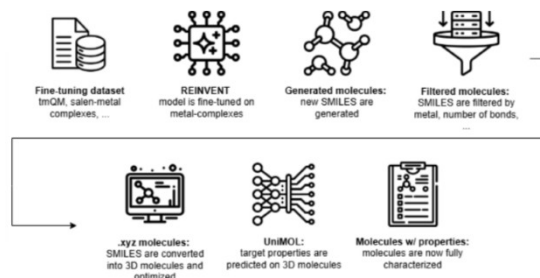
Results were analyzed through custom-developed interactive dashboards and analytical tools, enabling real-time visualization of molecular properties and structure.

Best candidates are selected for detailed analysis and lab synthesis.



Workflow Orchestration on HPC and Quantum Computing perspective

Orchestration of the complete pipeline on HPC infrastructure has been studied, to enable scalable processing of large molecular datasets and automated workflow through AiiDA framework.



An extensive assessment of available quantum generative AI tools was conducted, with a focus on approaches that can be reproduced with the current quantum constraints, leading to a **novel data encoding strategy of molecular structures in quantum circuits** paving the way for enhanced representation and analysis towards quantum utility.



Thank you