
Contribution ID: **78** Contribution code: **Board 26** Type: **Poster Presentation**

# Microscopic understanding of stability and adsorption/separation of CO2 from flue gas by MOFs in real industrial conditions

*Monday, May 20, 2024 7:10 PM (20 minutes)*

In light of the current environmental situation, reduction of anthropogenic CO2 emissions from carbon-intensive industries like power plants, cement, steel, or petrochemical industries become one of the most pressing issues to combat global warming. Shifting towards a low-carbon economy requires cost-effective carbon capture utilization or sequestration (CCUS) technology to be developed. Currently utilized amine-based absorption-regeneration process suffers from high energy penalties for solvent regeneration. In this regard, adsorption-based processes are considered promising alternatives for CCUS. Metal-organic frameworks (MOFs) are a widely studied class of porous adsorbents that offer tremendous potential, owing to their large CO2 adsorption capacity and/or high CO2 affinity. However, the performances of MOF-based CCUS technologies have not been fully evaluated in real industrial conditions. For example, the industrial flue gas contains CO2, N2, H2O, and traces of other contaminants, such as H2S, SO2, and NOx, which compete for different adsorption sites or might impact the stability of the adsorbent materials. Therefore, it is crucial to understand the competitive adsorption of the various components of the flue gas. From an experimental standpoint, such study is tedious and time consuming while molecular simulations provide a quicker route to understand their adsorption behavior and plausible degradation at the microscopic level. In this presentation, I will outline a systematic joint computational/experimental approach to evaluate the stability and CO2 capture performance of a series of MOFs in the presence of various impurities within the framework of MOF4AIR, a multidisciplinary H2020 EU project. A more detailed analysis will be provided for a few top-tier MOFs that were selected for large-scale deployment in the industrial post-combustion capture process.

Acknowledgement:

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 831975 (MOF4AIR project).

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**Session Classification:** Poster Session

**Track Classification:** Poster Presentations