

MOF-based QCM sensor for detecting and discriminating CH_{4}/CO_{2}

Malhotra, Jaskaran Singh; Kubus, Mariusz; Pedersen, Kasper S.; Andersen, Simon I.; Sundberg, Jonas

Publication date: 2023

Document Version Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA): Malhotra, J. S., Kubus, M., Pedersen, K. S., Andersen, S. I., & Sundberg, J. (2023). MOF-based QCM sensor for detecting and discriminating CH /CO. Poster session presented at 5th European Conference on Metal Organic Frameworks and Porous Polymers, Granada, Spain.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.

- · You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

DTU Offshore Danish Offshore Technology Centre



MOF-based QCM sensor for detecting and discriminating CH_4/CO_2



Collaborate!

Jaskaran Singh Malhotra^{1*}, Mariusz Kubus^{2,} Kasper S. Pedersen², Simon I. Andersen¹, Jonas Sundberg¹

Technical University of Denmark (DTU), 2800 Kongens Lyngby, Denmark (¹DTU Offshore; ²DTU Chemistry)

*jsima@dtu.dk

INTRODUCTION

- Among the most overlooked yet urgent environmental concerns is the fugitive emissions of CH₄ and CO₂ from gas pipelines, agriculture sector, wastewater treatment and landfills.¹
- We have developed a gas sensor based on a metal-organic framework (MOF) integrated in a quartz crystal microbalance (QCM) as a low-power and cost-effective solution for continuous monitoring of gas leaks.²



DTU

SENSORS&

FUNCTIONAL

MATERIALS

- [Cu(hfipbb)(H₂O)] is a 2-D MOF with narrow 1-D hydrophobic channels (5Å) connected via smaller gates (3Å) that shows selectivity towards CH4, and CO₂ compared to other atmospheric gases.³⁻⁴
- Difference in diffusivities of CH₄ and CO₂ into the MOF, enables discrimination based on multiple harmonic response of the QCM.²

SYNTHESIS

- Thin films of the MOF are directly grown on the gold electrode of 10 MHz quartz resonators via layer-by layer flow synthesis.
- First, a layer of thiol linker (16-mercaptohexadecanoic acid) is dip coated on the gold electrode.
- A peristaltic pump is used to alternate flows of ethanolic solutions of Cu²⁺ and the linker on the sensor in a custom-designed multi-channel flow cell.
- Powder X-ray diffraction confirms that the MOF-sensor film matches the calculated structure.



MOF-sensor

XRD

[Cu(hfipbb)(H₂O)]

[Cu(hfipbb)(H₂O)]

15

 2θ (degrees)

10

thin film

calculated

20

- Scanning electron microscopy shows disc-like crystals forming clusters.
- Atomic force microscopy shows average roughness features of ~1 μm



OUTLOOK

- > **MOF-based sensor.** Detects a range of concentrations of CH_4 and CO_2 (1-100 v/v% in N₂) with a limit of detection ~0.4%.
- Analyte discrimination. Enabled via frequency deviation of multiple harmonics.
- Practicality. The sensor shows a regenerative response. It works in air (under various humid conditions) at standard atmospheric conditions.
- > **Robustness.** Stable for months when stored at atmospheric conditions.
- Future work. Multivariate analysis to quantify responses from CH₄/CO₂ mixtures. Testing new MOFs for this application.

REFERENCES

- 1. Saunois et al. *Earth Sys. Sci. Data*, 2020, **12**, 1561-1623
- 2. Malhotra et al. ACS Sensors, 2023, available online (DOI: 10.1021/acssensors.3c01058)
- 3. Jiang et al. *Cryst. Engg. Comm.* 2009, **11** (5), 855
- 4. Sarkisov et al. *Chem. Mater.* 2020, **32** (23), 9849–9867

FUNDING

This research has received funding from the Danish Offshore Technology Centre