12 PhD positions in the EU Horizon Europe Marie Skłodowska-Curie DN-JD Project: SENNET (Porous Networks for Gas Sensing)

Applications are invited for 12 PhD positions ("Recruited Researchers - RR") to be funded by the Marie-Skłodowska-Curie Doctoral Network SENNET within the Horizon Europe Programme of the European Commission. SENNET is the "Porous Networks for Gas Sensing" project. SENNET will create disruptive sensor technology for indoor air quality by incorporating porous materials and sensor technology. The project has pooled the interdisciplinary and intersectoral expertise of leading members located in Belgium, Germany, France, Ireland, Moldova, Spain, UK and the Netherlands (**Figure 1**). The 12 SENNET RRs will not only receive state-of-the-art science/technology training but will also benefit from a unique soft-skills training programme. This will kick-start their careers as highly employable professionals in the EU and beyond.

Key dates

- 7 July 2022: Launch 12 PhD positions (RRs)
- 15 September 2022: Deadline for on-line application
- October 2022: Circulation list "SENNET Recruited Researchers" (some positions will be reopened if no suitable candidates will be identified)
- 1 March 2023 (at the latest): Targeted starting date for RR contracts

Key background info

Number of positions available
12 PhD Positions

Project type
SENNET is a MSCA DN-JD project (Doctoral Network - Joint Doctorate). Each recruited researcher will be enrolled in a doctoral programme in two EU Member States

Research Fields
Chemical Engineering, Computational Chemistry, Analytical chemistry, Materials Science, Inorganic Chemistry, Coordination Chemistry, High-throughput Experimentation, Micro- and nanofabrication, Electrical Engineering, Computer-aided design, Data Science, Chemometrics

Keywords
Sensors, gas, zeolites, MOF, VOC

Benefits and salary
The successful candidates will receive an attractive salary in accordance with the MSCA regulations for Recruited Researchers. The exact (net) salary will be confirmed upon appointment and is dependent on local tax regulations and on the country correction factor (to allow for the difference in cost of living in different EU Member States). The salary includes a living allowance, a mobility allowance and a family allowance (if applicable). The guaranteed PhD funding is for 36 months (i.e. EC funding, additional funding is possible, depending on the local Supervisor, and in accordance with the regular PhD time in the country of origin). In addition to their individual scientific projects, all fellows will benefit from further continuing education, which includes internships and secondments, a variety of training modules as well as transferable skills courses and active participation in workshops and conferences.

On-line Recruitment Procedure (see Appendix 1)
All applications proceed through the on-line recruitment portal on the https://sennet-project.eu/ website. Candidates apply electronically for one to maximum three positions and indicate their preference. Candidates provide all requested information including a detailed CV (Europass format obligatory) and motivation letter. During the registration, applicants will need to prove that they are eligible (cf. Recruited Researchers definition in Horizon Europe MSCA work programme 2021-2022, mobility criteria, and English language proficiency):

- Supported researchers must be doctoral candidates, i.e. not already in possession of a doctoral degree at the date of the recruitment.
- Researchers must be enrolled in a doctoral programme leading to the award of a doctoral degree in at least one EU Member State or Horizon Europe Associated Country, **and for Joint Doctorates in at least two**.

- Recruited researchers can be of any nationality and must comply with the following mobility rule: they must not have resided or carried out their main activity (work, studies, etc.) in the country of the recruiting beneficiary for more than 12 months in the 36 months immediately before their recruitment date.

The deadline for the on-line registration is **15 September 2022**. Prior to the recruitment, videoconferencing (or in person, when possible) interviews between the Supervisors and the candidates will be organized. The final decision on who to recruit is communicated no later than October 2022. The selected RRs are to start their research as quickly as possible (ideally prior to 01 March 2023).

Applicants need to fully respect three eligibility criteria (to demonstrated in the Europass cv):
Conditions of international mobility of researchers:
Researchers are required to undertake trans-national mobility (i.e. move from one country to another) when taking up the appointment. At the time of selection by the host organisation, researchers must not have resided or carried out their main activity (work, studies, etc.) in the country of their host organisation for more than 12 months in the 3 years immediately prior to their recruitment. Short stays, such as holidays, are not taken into account.
English language proficiency: Network fellows (RRs) must demonstrate that their ability to understand and express themselves in both written and spoken English is sufficiently high for them to derive the full benefit from the network training.

The 12 available PhD positions

(see **Figure 2** for interactions between RRs/WPs)

RR1: High-throughput (HT) screening & Rationalization of porous materials for selective VOC adsorption
Project Title: High-throughput (HT) screening & Rationalization of porous materials for selective VOC adsorption (WP1).
Host Institution: CNRS-Montpellier
Country: France
Supervisors: Prof. G. Maurin (CNRS-Montpellier); **Secondary Supervisors**: Prof. V. Van Speybroeck (UGENT), Stan van Gisbergen (SCM).
Objectives:

- HT screening of the IZA (zeolites) and CoreMOF 2019 (MOFs) databases using Monte Carlo simulations to identify the porous materials.
- QSPR analysis of the so-created database using advanced statistical tools (ANN, etc.)
- *In silico* design of novel MOFs with improved VOC adsorption performances assembling the key features identified in the previous step using an automated assembly of structure building units (AASBU) approach (case of MOF).

Short Description of Work & Expected Results:

- Creation of an unprecedented database listing the adsorption performances of porous materials with respect to VOCs
- Establishment of structure-adsorption property relationships using advanced statistical tools
- Prediction of novel porous materials with improved adsorption performances

Planned secondment(s):

- Host: UGENT, Prof. V. Van Speybroeck, Timing: year 2, Length: 6 months, Topic: Derivation of Accurate Force fields
- Host: SCM, Stan van Gisbergen, Timing: year 2, Length 2-3 months, Topic: Contributing to simulation software in a non-academic setting

Enrolment in Doctoral degree(s): Univ. Montpellier & UGENT
Candidate requirements:

- We are looking for a computational scientist with a good background in atomistic classical molecular simulations (Monte Carlo & Molecular Dynamics) and thermodynamics applied to material science.
- Very good skills in programing are also appreciated.

RR2: Characterisation of adsorption and dielectric and refractive index response of MOFs and zeolites
Project Title: Characterisation of adsorption and dielectric and refractive index response of MOFs and zeolites (WP1)
Host Institution: Ghent University
Country: Belgium
Supervisors: Prof. V. Van Speybroeck (Ghent University) Prof. L. Vanduyfhuys (CNRS-Montpellier); **Secondary Supervisors**: Prof. G. Maurin (CNRS-M), Stan van Gisbergen (SCM)
Objectives:

- Accurate prediction of adsorption isotherms and selectivity of nanoporous materials towards various VOCs
- Accurate prediction of the dielectric constants and refractive index of nanoporous materials loaded with VOCs

Short Description of Work & Expected Results:

- Construction of accurate material specific force fields (FFs) and/or ab initio trained machine learning potentials (MLPs) for 50 of the most promising materials for each VOC as identified by CNRS-Montpellier
- Use these FFs/MLPs for the simulation of single- and multicomponent isotherms for the most promising 50 materials for each VOC identified by CNRS-Montpellier
- Calculation of the dielectric constant and refractive index response for the 10 most promising materials for each VOC identified as function of their guest (VOC/water) loading using ab initio techniques such as DFT

Planned secondment(s):

- Host: CNRS-Montpellier, Prof. G. Maurin, Timing: year 1, Length: 6 months, Topic: High-throughput screening
- Host: SCM, Stan van Gisbergen, Timing: year 2, Length 2-3 months, Topic: Contributing to simulation software in a non-academic setting

Enrolment in Doctoral degree(s): UGENT & Univ. Montpellier

Candidate requirements:

- We are looking for a computational scientist with a good background in atomistic molecular simulations, quantum mechanics, statistical physics and thermodynamics applied to material science.
- Experience with molecular simulation software (LAMMPS, DLPOLY, RASPA, Gaussian, VASP, CP2K, …) and coding (Python, C, …) is an advantage.
- You have a pro-active working style, the willingness to look beyond the borders of your own discipline and a strong motivation to work in a multidisciplinary team. You are highly motivated to become an independent researcher.
- You have excellent communication skills and have a strong motivation to collaborate with other researchers, within the CMM, the SENNET consortium and our networks.
- You have or will soon obtain a master's degree of a university or international equivalent in the field of Chemistry, Chemical Engineering, Physics, Physical Engineering or a related field

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RR3: Synthesis of Metal-organic frameworks for the detection of VOCs

Project Title: Synthesis of Metal-organic frameworks for the detection of VOCs (WP2)

Host Institution: CAU

Country: Germany

Supervisors: Prof. N. Stock (Ghent University); **Secondary Supervisors**: Prof. J. Denayer (VUB), Karl Petter Lillerud (ProfMOF)

Objectives:

- Vapour- phase and solution-based synthesis of pure and mixed-linker MOFs with finely tuned pore openings and pore surface chemistry

Short Description of Work & Expected Results:

- The synthesis efforts in the Stock group will focus on Al-, Zr- and Zn-based MOFs due to their chemical and thermal stabilities and our own experience with these materials. Mixed-ligand Al- and Zr-MOFs with known structure type will be synthesized first in order to study synergistic effects triggered by certain combinations of functional groups on the linkers, which will enhance the selectivity of analytes of interest.

Planned secondment(s):

- Host: VUB, Prof. J. Denayer, Timing: year 2, Length 6 months, Topic: Characterization through high-resolution adsorption measurements
- Host: ProfMOF, Karl Petter Lillerud, Timing: year 3, Length 2 months, Topic: Upscaling of MOF synthesis. Working in a non-academic setting.

Enrolment in Doctoral degree(s): CAU & VUB

Candidate requirements:

- We are looking for a scientist with a very good background in materials synthesis and characterisation, especially using X-ray diffraction methods. Skills in structure determination from powder diffraction data using the Rietveld method as well as sorption measurements are also appreciated.

RR4: Synthesis of nanosized zeolites for the detection of VOCs

Project Title: Synthesis of nanosized zeolites for the detection of VOCs (WP2)

Host Institution: CNRS

Country: France

Supervisors: Prof. S. Mintova (CNRS-Caen); Dr. M. Denoual (CNRS-Caen); **Secondary Supervisors**: Prof. I. Naydenova (TDUB), George Lamy au Rousseau (STARNAV)

Objectives:

- To develop novel or optimize the available synthesis approaches towards preparation of zeolite nanoparticles with variable pore openings s.
- Functionalization of the zeolite nanoparticles by direct synthesis or post-synthesis approaches towards improved VOC detection and selectivity.
- In situ IR characterization of adsorption and desorption of single VOC and mixtures in zeolite and MOF thin films deposited on sensor devices.
- In situ XRD characterization of adsorption and desorption of single VOC and mixtures in zeolite and MOF powders.

Short Description of Work & Expected Results:

- The best-performing nanosized zeolites will be identified for selective VOC adsorption. The nanosized zeolites have to fit the requirements for the detection of VOCs under realistic operating conditions. The effectiveness of the nanozeolites will depend on the (i) capacity; (ii) kinetics; (iii) selectivity; and (iv) stability/regeneration, as well as on the green method of their preparation.

Planned secondment(s):

- Host: TDUB, Prof. I. Naydenova, Timing: year 2, Length: 6 months, Topic: Incorporation of zeolite nanoparticles in photonic sensors.
- Host: Starnav, George Lamy au Rousseau, Timing: year 3, Length 2 months, Topic: Sensor incorporation of nanosized zeolites, developing
  data processing tools, and looking into valorisation opportunities related to end-product development. Working in a non-academic setting.

Enrolment in Doctoral degree(s): Univ. Caen & Tech. Univ. Dublin

Candidate requirements:

- Must have a master degree in chemistry, chemical engineering or material science.
- A relevant experience in physical chemistry, materials chemistry is mandatory.
- We are looking for a highly motivated candidate to be the link between two teams working in material science and sensors engineering.
- Efficient in oral and written communications.
- Mastery of oral and written English is mandatory.

RR5: A dynamic method for measuring multicomponent adsorption equilibria at ultra-low concentration

Project Title: A dynamic method for measuring multicomponent adsorption equilibria at ultra-low concentration (WP3)

Host Institution: VUB

Country: Belgium

Supervisors: Prof. J. Denayer (VUB); **Secondary Supervisors**: Prof. M. Thommes (FAU), Dr. Michelle Mercer (Hiden)

Objectives:

- The development of an experimental method that allows the study of competitive adsorption with complex mixtures at very low concentrations.
- The use of this method to screen new adsorbent materials (zeolites and MOFs) for sensing applications.
- The determination of adsorption parameters, required for the signal processing task and the validation of molecular modelling results.

Short Description of Work & Expected Results:

- This RR project aims at the development and use of dynamic methods to determine multicomponent adsorption equilibria of mixtures of selected VOCs at very low concentrations. Inverse pulse chromatography will be used for a first screening of low coverage adsorption properties for pure components.

Planned secondment(s):

- Host: FAU, Prof. M. Thommes, Timing: year 2, Length 6 months, Topic: Characterization using single-component adsorption methods.
- Host: Hiden, Dr. Michelle Mercer, Timing: year 2, Length 2-3 months, Topic: Training in the Integral Mass Balance technique to study multicomponent adsorption. Working in a company environment.

Enrolment in Doctoral degree(s): VUB & FAU

Candidate requirements:

- It is expected that the successful candidate has a master degree in chemical engineering, bio-engineering sciences, chemistry, or a related field
- Excellent knowledge in physical chemistry, mass and heat transfer and thermodynamics is expected
- The successful candidate is interested in data analysis and computer modelling
- The successful candidate has good experimental skills
- The successful candidate has excellent communication skills and a strong motivation to collaborate with other researchers within the SENNET consortium
- Excellent oral and written English language skills are mandatory.

RR6: Targeted characterization and adsorption properties of MOF and zeolitic adsorbents for gas sensing

Project Title: Targeted characterization and adsorption properties of MOF and zeolitic adsorbents for gas sensing (WP3)

Host Institution: FAU

Country: Germany

Supervisors: Prof. M. Thommes (FAU); **Secondary Supervisors**: Prof. S. Mintova (CNRS-Caen), Dr. Michelle Mercer (Hiden)

Objectives:

- Develop novel, application-directed characterization methodologies for surface and pore structure characterization of MOFs and zeolites
- Systematic, experimental assessment of adsorption behaviour of VOCs of interest and water in MOFs and zeolites. Adsorption studies will be conducted with dedicated static and dynamic methods.
- Assessing structure-property relationships. Correlating surface and pore structure with adsorption behaviour of VOCs and water.

Short Description of Work & Expected Results:

- Advanced adsorption-based characterization for the behaviour of the selected VOCs will be developed. The methodology will be based on combining the adsorption behaviour of vapours (which are sensitive to both pore surface functionality and pore structure) at various temperatures with adsorption of inert gases (e.g., argon) to only assess textural properties, combined with statistical mechanics (e.g., mean field DFT) for data analysis.

Planned secondment(s):

- Host: CNRS-Caen, Prof. S. Mintova, Timing: year 2, Length 6 months, Topic: Synthesis of porous materials synthesis (nanozeolites).
- Host: Hiden, Dr. Michelle Mercer, Timing: year 2, Length 2-3 months, Topic: Training in high-resolution gravimetric adsorption measurements.

Enrolment in Doctoral degree(s): FAU & Univ. Caen

Candidate requirements:

- It is expected that the successful candidate has a master degree in chemical engineering, chemistry, materials science or a related field
- Excellent knowledge in physical chemistry is expected
- The successful candidate has excellent communication skills and a strong motivation to collaborate with other researchers within the SENNET consortium
- Excellent oral and written English language skills are mandatory.

RR7: Fabrication of MOF- and zeolite-functionalized resistive sensors, sensor arrays, and pre-concentrators

Project Title: Fabrication of MOF- and zeolite-functionalized resistive sensors, sensor arrays, and pre-concentrators (WP4)

Host Institution: CAU

Country: Germany

Supervisors: Prof. R. Adelung (CAU); **Secondary Supervisors**: Prof. R. Ameloot (KUL), Andreas Walte (Airsense)

Objectives:

- Decoration of compatible MOF-structures on metal oxide nanowire sensors fabricated by 3D printing. MOFs and zeolites will either be wet
chemically deposited via nanoparticles or directly grown on adequate metal oxides like ZnO or TiO2.
- MOF-functionalised porous graphene networks used as pre-concentrators for specific VOCs
- Integration of sensors with MOF- or zeolite-functionalised pre-concentrators for specific VOCs
- Integration of multiple, partially selective sensors into one sensor array, equipped with pre-concentrator and custom electronics.

Short Description of Work & Expected Results:

- Various metal microparticles will be printed via direct ink writing. Direct ink writing can produce these particles with a thickness of 100-1000 µm.
- Multiple sensor systems will be printed and included into an array to be cross-related to obtain the best possible selectivity.
- A channel system with inlets decorated with zeolites and MOFs will act as a retention agent depending on the molecules size and the pores. A MOF- or zeolite-functionalised porous graphene structure will allow for rapid heating to release the adsorbed VOCs.

Planned secondment(s):

- Host: KUL, Prof. M. Kraft, Timing: year 2, Length 6 months, Topic: Cleanroom training and sensor fabrication via various patterning methods.
- Host: Airsense, Andreas Walte & Bert Ungethüm, Timing: year 3, Length 2-3 months, Topic: Sensor integration and evaluation, training in the assembly of prototypes, programming sensor read-out software. Working in a company environment.

Enrolment in Doctoral degree(s): CAU & KU Leuven

Candidate requirements:

- The ideal candidate will have a profile containing Materials Science, with special focus on semiconductor technology, fabrication technology and interface chemistry and physics.
- Additional candidate profiles may include a background in physics, chemistry and mechanical engineering.

RR8: Evaluation of sensitivity, selectivity and stability of MOF- and zeolite-functionalized resistive sensors, sensor arrays, and pre-concentrators for the detection of VOCs mixtures

Project Title: Evaluation of sensitivity, selectivity and stability of MOF- and zeolite-functionalized resistive sensors, sensor arrays, and pre-concentrators for the detection of VOCs mixtures (WP4)

Host Institution: TUM

Country: Moldova

Supervisors: Prof. O. Lupan (TUM); **Secondary Supervisors**: Prof. R. Adelung (CAU), Bert Ungethüm (Airsense)

Objectives:

- Development of a testing setup for low concentration VOC gas sensing experiments for mixed atmospheres in defined concentrations
- Electrical and Chemical-electrical evaluation of sensor arrays down to the 10 ppb range
- Implementation of multiple sensor arrays readouts for cross-platform sensing and correlated signal evaluation
- Long-term stability and sensor drift tests for quality assessment

Short Description of Work & Expected Results:

- An existing gas-sensing setup will be modified to sense low concentrations (down to the ppbrange) of the proposed VOC as well as mixtures of these compounds with both air and other known VOCs like acetone and ethanol.
- A measurement stage will be implemented to test sensors and arrays fabricated at CAU at different temperatures and atmosphere compositions.

Planned secondment(s):

- Host: CAU, Prof. R. Adelung, Timing: year 1, Length 6 months, Topic: Sensor fabrication via inkjet deposition and other patterning methods.
- Host: Airsense, Andreas Walte & Bert Ungethüm, Timing: year 3, Length 2 months, Topic: Programming sensor read-out software.

Enrolment in Doctoral degree(s): TUM & CAU

Candidate requirements:

- The ideal candidate would have a background in Applied Physics: Physics and technology of materials; Physics of nanosystems and nanotechnology or a background as a Solid State Electronics engineer: nano-microelectronics and optoelectronics; technology and components in electronics; solid state electronics; biomedical equipment and devices.

RR9: Coupled MEMS resonant sensors exploiting the mode-localization effect for the detection of VOCs

Project Title: Coupled MEMS resonant sensors exploiting the mode-localization effect for the detection of VOCs (WP5)

Host Institution: KU Leuven

Country: Belgium

Supervisors: Prof. M. Kraft (KU Leuven); **Secondary Supervisors**: Prof. R. Adelung (CAU), T. Dieryckx (Voxdale)

Objectives:

- Design, fabricate and test novel MOF-functionalised resonators for gravimetric VOC sensing.
- To investigate and employ this approach for gas sensing applications.
- To demonstrate the first coupled resonator based on this approach.

Short Description of Work & Expected Results:

- Design study (using Comsol and Coventorware) of a coupled resonator with thermal actuation and piezoresistive sensing. Fabricate several prototypes in the KU Leuven Nanocentre using a fabrication process based on DRIE of SOI wafers.
- Construction of suitable interface circuits with off-the-shelf components.
- Coating of the resonators with selected MOFs supplied by RR3 or RR11.

Planned secondment(s):

- Host: CAU, Prof. R. Adelung, Timing: year 2, Length: 6 months, Topic: Resistive sensor design study and comparison with MEMS
- Host: Voxdale, T. Dieryckx, Timing: year 3, Length 2-3 months, Topic: integration of sensors into modules suitable for real-world testing and/or the creation of an interface for data collection.

Enrolment in Doctoral degree(s): KU Leuven & CAU

Candidate requirements:

- The ideal candidate should have a background and Master degree in micro- and nanosystems, electrical or mechanical engineering, applied physics, material science or a related discipline. Experience in micro-fabrication and working in a cleanroom is desirable.

RR10: A metal-organic framework capacitive sensor array as an electronic nose for volatile organic compound detection

Project Title: A metal-organic framework capacitive sensor array as an electronic nose for volatile organic compound detection (WP5)

Host Institution: KU Leuven

Country: Belgium

Supervisors: Prof. R. Ameloot (KU Leuven); **Secondary Supervisors**: Prof. I. Naydenova (TDUB), T. Dieryckx (Voxdale)

Description of the organizational unit:

The Ameloot group is part of the KU Leuven Center for Membrane Separations, Adsorption, Catalysis, and Spectroscopy (cMACS), which counts 6 PIs and >100 members. The study of porous materials, membranes, films and their interfaces forms the core of the research at cMACS. In this context, our group studies different flavors of porous and hybrid matter and has been awarded ERC Starting and Consolidator Grants on this topic. For more information, please refer to http://amelootgroup.org/ and https://twitter.com/AmelootGroup.

Objectives:

- Demonstrate a novel concept to enable selective VOC sensors based on metal-organic frameworks (MOFs)
- Measure and understand VOC adsorption and diffusion in MOF sensor coatings
- Fabricate a MOF sensor array that functions as an 'electronic nose'
- Data and performance analysis of the sensors and sensor arrays

Short Description of Work & Expected Results:

Detecting and monitoring volatile organic compounds (VOCs) is an important task with applications ranging from disease diagnosis via breath analysis to monitoring exposure to toxic chemicals. However, in all such applications, selectively measuring specific VOCs is challenging due to their low concentrations and the presence of a multitude of interfering compounds. Since current miniature sensors cannot efficiently distinguish between VOCs, there is a need for a novel technology capable of distinguishing a VOC of interest from a complex background.

This RR project will address this challenge by bridging the worlds of porous crystalline materials and sensor technology. For the first time, kinetic selectivity in the nanopores of MOFs will be leveraged to mimic nature's approach to olfaction and enable selective sensing. You will focus on developing a MOF-based electronic nose integrating a new sensing strategy based on the system's transient behavior. This application-oriented project includes the characterization of adsorption and diffusion of probe molecules in MOFs, the efficient integration of MOF films in a suitable e-nose architecture, and analyzing their performance towards target atmospheres via multi-component sensing studies and chemometric data analysis. A range of in-situ characterization protocols (gravimetric, optical, and capacitive transduction) combined with advanced in-house-built dosing systems will be used to study the sensing properties and evaluate the e-nose performance.

This PhD position will work closely together with three postdoctoral researchers and one PhD student currently working on complementary aspects of this promising project through the ERC project 'KISSIES'. Through your tasks in the project, you will work closely with scientists and engineers with expertise in materials synthesis, gas adsorption and diffusion, the characterization of porous and crystalline materials, etc. As a PhD candidate, you will write and publish scientific articles, actively participate in international and national congresses/consortium meetings and develop your soft- and technical- skills via international research stays and (doctoral school) training courses, with the aim of writing a doctoral dissertation.

Planned secondment(s):

- Host: TDUB (Type: University; Location: Ireland), Prof. I. Naydenova, Timing: year 2, Length: 6 months, Topic: Incorporation of MOF coatings in photonic sensors.
- Host: Voxdale (Type: Engineering company; Location: Belgium), T. Dieryckx, Timing: year 3, Length 2-3 months, Topic: integration of sensors into modules suitable for real-world testing and/or the creation of an interface for data collection

Enrolment in Doctoral degree(s): KU Leuven & TDUB

Candidate requirements:

- A candidate with a passion for novel porous materials, microfabrication, and measurement technology (incl. data science)
- A motivated candidate with a strong academic track record and a degree in Materials Chemistry, Physics, or a related field in Science and Engineering.
- A candidate willing to tackle a highly interdisciplinary application-oriented project
- A team player willing to work as part of an interdisciplinary group
- A candidate with an interest in literature reviewing, scientific writing, presenting research to an expert audience.
- Previous demonstrations of out-of-the-box thinking. Bonus points if you consider yourself a 'maker' and practical problem solver, we appreciate what you are doing!
- Since we are a highly international team, proficiency in both written and spoken English is non-negotiable.
- Since the research consortium spans multiple disciplines, the ability to communicate clearly across subject boundaries is essential

Please consider applying if you have several of the following skills:

- Experience in nanoporous materials synthesis and characterization (required)
- Experience in microfabrication
- Experience in data science, chemometrics, and information extraction from chemical data
- Other skills that you think are important (please explain in your cover letter).

Interested?

For more information about this job opportunity, please contact Prof. Rob Ameloot (rob.ameloot@kuleuven.be) via email and mention "PhD position MOF e-nose" in the subject line.

Preferred starting date: September – December 2022

RR11: Development of highly sensitive diffractive optical sensors for detection of VOCs

Project Title: Development of highly sensitive diffractive optical sensors for detection of VOCs (WP5)

Host Institution: TDUB

Country: Ireland

Supervisors: Prof. I. Naydenova (TDUB); **Secondary Supervisors**: Prof. R. Ameloot (KUL), Dr. Y. Ponomarev (Analog Devices)

Objectives:

- To develop surface holographic sensors for VOCs based on MOF- or zeolite-functionalised surface holograms.
- To develop holographic sensors for VOCs based on volume holograms functionalised by MOFs or zeolites in the polymer layer.
- To model and optimize the sensitivity of hybrid opto-mechanical sensors and to examine/validate the model by comparison to experiments.
- To fabricate a proof-of-concept hybrid opto-mechanical holographic sensors functionalised MOFs or zeolites and evaluate their performance.

Short Description of Work & Expected Results:

- Holographic structures of surface or volume holograms will be functionalised by coating/impregnating with either MOFs or zeolites and their sensing properties will be tested and optimised. Testing will include characterisation of sensitivity, selectivity, stability, signal-to-noise ratio, reversibility, response time.

Planned secondment(s):

- Host: KUL, Prof. R. Ameloot, Timing: year 2, Length 6 months, Topic: Characterisation of layers with integrated MOF materials.
- Host: Analog Devices, Dr. Y. Ponomarev, Timing: year 3, Length 2-3 months, Topic: Sensor testing in an industrial R&D lab.

Enrolment in Doctoral degree(s): TDUB & KUL

Candidate requirements:

- A motivated candidate with a strong academic track record and a degree in Physics, Chemistry or a related field in Science and Engineering. The project requires excellent knowledge in Optics/Photonics and knowledge in Materials Science.
- A team player willing to work as part of an interdisciplinary consortium across multiple universities.
- A candidate with an interest in literature reviewing, scientific writing, presenting research to an expert audience.
- Demonstration of out-of-the-box thinking and personal initiative is desirable.
- Since we are a highly international team, proficiency in both written and spoken English is mandatory.
- Since the research consortium spans multiple disciplines, the ability to communicate clearly across subject boundaries is essential.

RR12: Data processing to optimize the fabrication of MOFs and zeolites sensor arrays

Project Title: Data processing to optimize the fabrication of MOFs and zeolites sensor arrays (WP1)

Host Institution: University of Barcelona

Country: Spain

Supervisors: Prof. A. Gutierrez-Galvez (University of Barcelona); **Secondary Supervisors**: Prof. R. Ameloot (KUL), Dr. M. Van Poppel (VITO)

Objectives:

- Evaluating the different materials to be combined in a sensor array.
- Guiding the calibration of fabricated sensors by designing a set of experiments considering target gases as well as interfering compounds.
- Building calibration models for the final sensors and arrays of the project.
- Building data processing methods to improve the stability of the sensors response over time by counteracting sensor drift.

Short Description of Work & Expected Results:

- The selection of materials for sensor arrays will be performed via statistical and information theoretic methods that measure the complementarity of the array response to the target VOCs. A set of experiments will be designed to obtain a comprehensive response of the sensors and sensor arrays to combinations of target and common interfering gases at different mixtures.

Planned secondment(s):

- Host: KUL, Prof. R. Ameloot, Timing: year 3, Length: 6 months, Topic: MOF synthesis and sensor testing.

- Host: VITO, Dr. M. Van Poppel, Timing: year 3, Length: 2 months, Topic: Analysis of environmental sensing data with real-world settings

Enrolment in Doctoral degree(s): BARC & KUL

Candidate requirements:

- We are looking for a highly motivated physicist/engineer with a master in data science and a good background in instrumentation.
- The candidate should have very good programming skills and proven experience in Python, R, or MATLAB.
- Proficient levels of spoken and written English are required
- Good group working skills are also needed for this position

DN-JD SENNET project abstract and key project information

According to a recent study in Europe and the US[1], air pollution kills as many as 10 million people every year, making it considerably more lethal than COVID-19. It has been described as a 'pandemic in slow motion', with the people living in polluted areas much more likely to suffer from chronic illnesses [2]. While outdoor air pollution usually grabs the headlines, the effects of indoor air pollution – most often felt by women, children and the elderly, especially in less-developed parts of the world – can frequently be worse.[3] Household items like carpets, paints, and furniture release volatile organic compounds (VOCs), which not only cause discomfort, but can lead to debilitating or even fatal respiratory diseases and cancers[4].

But before we can tackle the problem, we need to be able to measure VOC concentrations with high spatial and temporal resolution, and if we are going to do this on a global scale, the sensors will have to be low-cost, reliable and small. Air-quality sensors available today produce data that is often questionable, due to the measurement approach itself or their susceptibility to environmental parameters.[5,6] Metal oxide semiconductor sensors, for example, cannot usually distinguish between a harmful VOC and harmless compounds (e.g., water vapour, food aromas, metabolic side-products such as ethanol and acetone). Indeed, selectively measuring a single, harmful VOC is very challenging, because of the low concentration of the analyte and the multitude of interfering compounds that are present in indoor air.

SENNET's aim will be to develop new, high-quality, low-cost miniature sensors and sensor arrays for the selective detection of VOCs. Our approach is based on exploiting the adsorption properties of two tuneable porous-material families: metal-organic frameworks (MOFs) and zeolites. What makes SENNET different to the projects that have come before, is that we will combine the study of these porous crystalline materials with advances in sensor technology. These are two subjects that have so far existed separately.

The market for indoor air-quality monitors is expected to exceed €4 billion by 2022.[7] This market is fragmented into SMEs and multinationals offering a range of different products. Several European companies are major players, for example,[8] Bosch Sensortec, AMS, Analog Devices*, Sensirion, Alphasense, and Airsense Analytics* (Associated Partners in SENNET*). However, Europe has a shortage of the multidisciplinary researchers and technologists needed to develop new materials and sensors.[9,10] For this reason, we are proposing to establish a training network, rather than a research-only project.

Breakthrough materials. MOFs and zeolites are crystalline, porous network materials. Whereas zeolites are inorganic aluminosilicates containing extra-framework cations, MOFs are hybrid solids that consist of inorganic nodes connected by multitopic organic molecules. Both classes of material have uniform pores with dimensions comparable to the size of the VOCs to be detected and have high surface areas (up to 6000 m^2 g^{-1}). Because of their chemical and structural characteristics, MOFs and zeolites can capture VOCs even at trace concentrations.[11] Moreover, the adsorption preference (or selectivity) can be tuned by changing the nature of the framework. Although these adsorption properties are potentially very promising for VOC sensors, the integration of MOFs or zeolites into real devices has been largely overlooked. Firstly, due to a lack of systematic knowledge about which of the many different MOFs or zeolites would be best suited to adsorb a particular VOC from the air, and, secondly, the lack of suitable methods to integrate these materials with a sensor technology, e.g., coating deposition and signal transduction.

Taking up the challenge. SENNET will address these challenges by combining expertise from fundamental chemistry all the way through to sensor engineering, resulting in the scientific objectives (SOs) outlined below . The overall approach is to combine multiple sensor elements coated by a porous material that displays cross-selective but different adsorption behaviour. The nature and concentration of the target VOC will be determined from the combined response of all the sensor elements through a multivariate calibration approach borrowed from chemometrics. The focus will be on the priority risk VOCs determined by the World Health Organization, *i.e.,* tetrachloroethylene, formaldehyde and benzene.

Scientific objectives. The project's five Scientific Objec-tives (SOs) are defined below:

(SO1) Because of the large numbers of MOFs (> 10,000) and zeolites (> 240), and their numerous multicomponent adsorption behaviours, an efficient screening approach is needed. High-throughput computational approaches will be developed to tackle this problem and identify structure-adsorption property relationships.

(SO2) The predicted behaviour must be validated by **experimental adsorption tests for both single components and complex mixtures** to fully understand the behaviour of the materials in indoor air.

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1 https://doi.org/10.1016/j.envres.2021.110754

2 National Geographic, March 16, 2021

3 https://www.mana.md/indoor-air-vs-outdoor-air/

4 *Arch. Toxicol.* **84**, 423–446 (2010).

5 *Nature* **535**, 29–31 (2016).

6 https://www.epa.gov/air-sensor-toolbox/evaluation-emerging-air-pollution-sensor-performance

7 https://www.marketsandmarkets.com/Market-Reports/indoor-air-quality-monitor-market-109800608.html

8 Zoominfo (www.zoominfo.com). Note: several companies have multiple business units, apart from sensors.

9 Bosch Sensortec currently has 75 technology vacancies (22 Sep 2021): https://www.bosch.de/en/career/job-offers/?searchTerm=%22Bosch%20Sensortec%22&sortBy=releasedDate

10 https://www.cedefop.europa.eu/files/nanotechnology_proceedings_undedited.pdf

11 Ameloot and co-workers, *Chem. Sci.* **7**, 5827–5832 (2016).

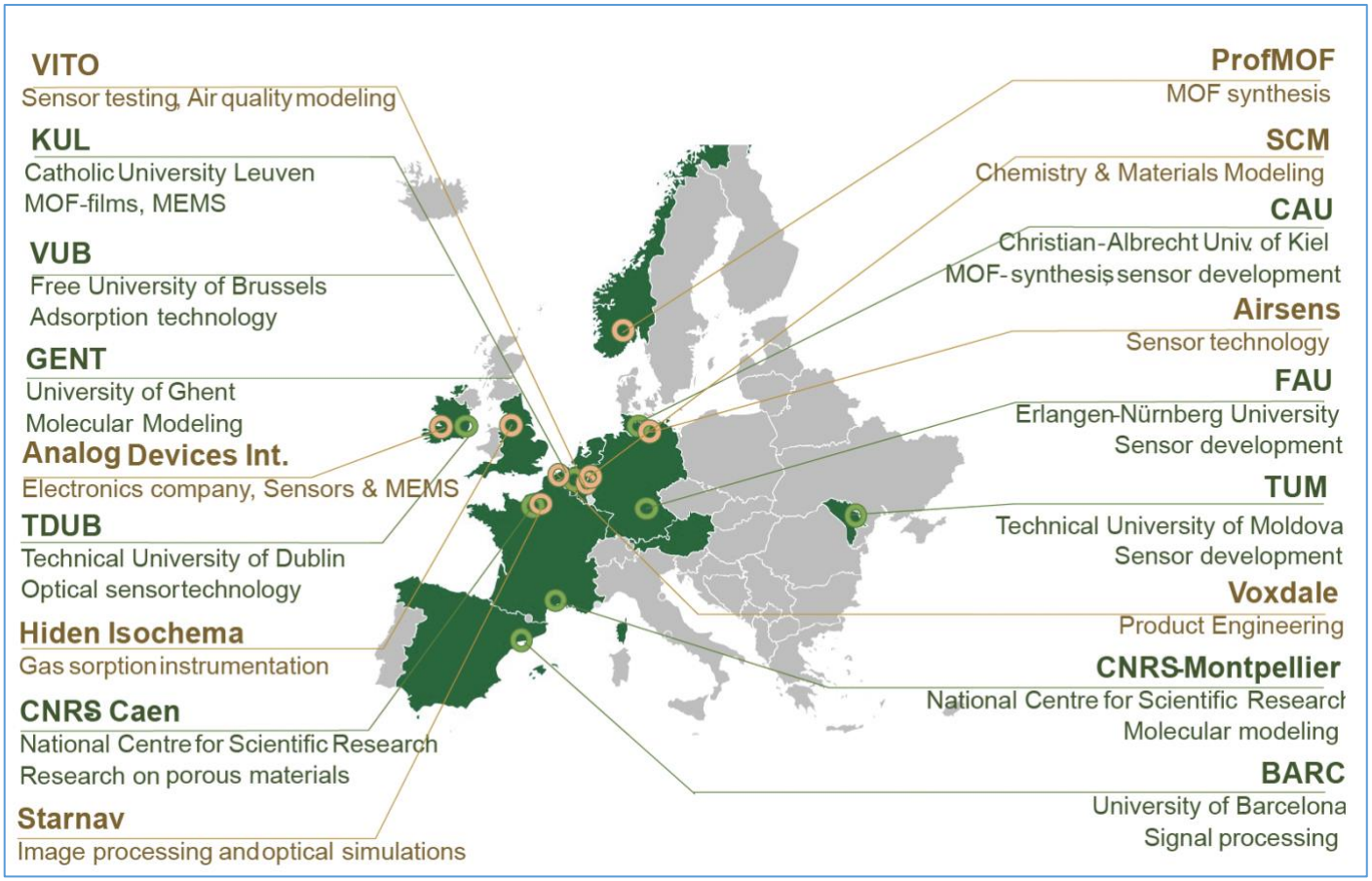
(SO3) Synthesis of MOFs and zeolites and fine-tuning of their properties to obtain the required mixed-component adsorption behaviour, based on the identified structure-adsorption property relationships. The materials will be prepared in a form that facilitates their integration in sensors.

(SO4) Sensor fabrication and testing based on the most promising MOFs and zeolites. New fabrication approaches will be explored and the testing will involve real-world conditions. Different strategies to transduce the VOCs' adsorption characteristics into a measurable signal will be benchmarked.

(SO5) Signal-processing methods will be developed to calibrate the sensors and sensor arrays and to pre-vent non-selective or drifting signals as a result of temperature, relative humidity, or interfering com-pounds.

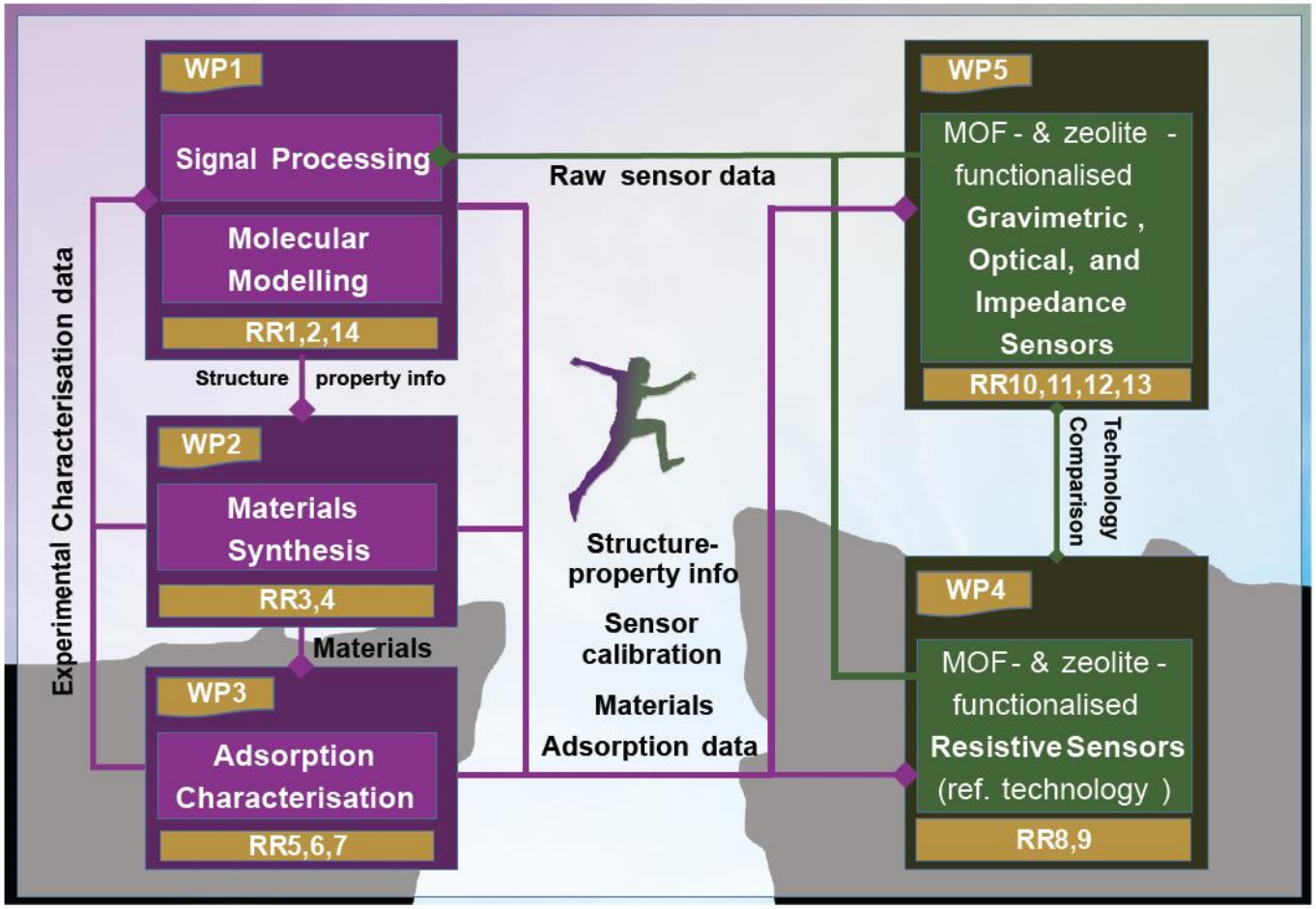
Research & Innovation excellence based on a top-flight consortium. SENNET is a doctoral training network involving the very best of Europe's research teams focused on MOF and zeolite materials and sensors see **Figure 1**). The Beneficiaries include top-ranked universities like KU Leuven, FAU Erlangen Nuernberg, Universitat de Barcelona and the Centre National De La Recherche Scientifique (CNRS). Among the Associated Partners there are dynamic SMEs like Airsense Analytics, Voxdale, and Hiden Isochema working on air-quality monitoring, sensor integration, product development, and adsorption measurement technology, and European industry like Analog Devices, a leader in sensor design and large-scale fabrication.

Figure 1: SENNET Consortium



SENNET's five scientific objectives (SOs) translate into five work packages (**WPs1–5**). All the WPs are fully interwoven and provide feedback to each other to select, optimise, integrate and test the MOFs and zeolites in the context of selective VOC sensing. Despite the collaborative nature of the project, all the tasks will be initiated in parallel once the RRs have been recruited. An overview of these WPs and which SOs they address is given in **Table 1.1b**. The scientific tasks are complemented by dedicated WPs dealing with Training activities (**WP6**), Exploitation, communication & dissemination (**WP7**), and Project management & recruiting (**WP8**). A schematic of the SENNET WPs, RRs and internal interactions is given in **Figure 2**.

Figure 2: SENNET Work Packages and RRs



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Appendix 1: Recruitment Procedure and Principles

A SENNET recruitment webpage is put on-line (July 2022), as part of the SENNET project website: https://sennet-project.eu/

Key dates

- 7 July 2022: Launch 12 PhD positions (RRs)
- 15 September 2022: Deadline for on-line application
- October 2022: Circulation list "SENNET Recruited Researchers" (some positions will be reopened if no suitable candidates will be identified)
- 1 March 2023 (at the latest): Targeted starting date for RR contracts

Applications are made through an on-line, eligibility-proof form on the SENNET recruitment webpage. The candidates apply for a maximum of three specific RR positions and list their order of preference. After interviewing (through videoconferencing means or in person, if possible) the candidates, the corresponding Supervisors provide the names of their preferred candidates to the project's Supervisory Board. The final list of selected researchers will be discussed and approved by the Supervisory Board. Final ranking of applicants will be made by the Supervisory Board, who might conduct additional selection interviews with the most suitable candidates (through videoconferencing means or in person, if possible). The final appointment of each selected researcher will be subject to approval by the two Doctoral Schools in which the candidate is supposed to be enrolled in doctoral programmes.

All details concerning the recruitment-procedure principles are communicated on the on-line application portal, so that potential RRs know exactly what to expect and are stimulated to apply. All recruitment is in line with the European Charter for Researchers, providing the overarching framework for the roles, responsibilities of both researchers and employers. The Code of Conduct for the Recruitment of Researchers functions ensures that the selection procedures are transparent and fair.

The recruitment strategy of SENNET fully complies with the Code of Conduct definition of merit. For example, merit is not just measured by a researcher's grades, but on a range of evaluation criteria, such as teamwork, interdisciplinary knowledge, soft skills and awareness of the policy impact of science.

The Supervisory Board has members of each gender and considers the promotion of equal opportunities and gender balance as part of the recruitment strategy. Also, in view of the RRI principles, special efforts are made to attract women and RRs from new EU Member States.

SENNET aims at a participation of 50% female RRs in the network. Researchers are employed on fixed-term contracts and are registered as staff candidates for PhD degrees. Therefore, they are entitled to pension contributions, paid holidays, and other benefits as governed by the universities and industrial companies.

For any inquiries regarding the recruitment procedure, please send an email to info@sennet-project.eu