Helmholtz - OCPC - Programme 2017-2021
for the Involvement of Postdocs in Bilateral Collaboration Projects with China

PART A

Title of the project: Metal organic framework membranes for critical industrial gas separations

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Description of the project (max. 1 page)**:**
Olefin/paraffin separations are critically important industrial gas separations, carried out on a massive scale globally. Two of the most common are propane/propylene, and ethane/ethylene, as these provide the crucial polymer precursors propylene and ethylene, with current global production in excess of 200 million tonnes annually, or around 30kg for every person on the planet[1]. The energy consumption globally in carrying out these separations currently (using large-scale cryogenic distillation) is a major contributor to the overall energy consumption and greenhouse gas emissions of the petrochemical sector. These two gas separations are responsible for approximately 0.3% of total global energy consumption. The chemical sector in general is critically important to both Europe and China. In Europe, the chemical sector underpins major export earning sectors including automotive, food and drink, and general manufacturing as a supplier of key input materials, while at the same time the chemical sector is itself a major employer, source of investment, and adds considerable value to the economy – 299.4b € in value added to the European economy in 2015, compared to 200.4b € from the automotive sector[2]. Globally, the chemical sector is growing but with the majority of all growth in China, where the industry grew at 10.7% average annual growth rate over the period 2007 – 2017.

Recent developments in metal organic framework materials show that it should be possible to use easy-to-synthesise porous materials including ZIF-8 as membranes, with single stage molecular selectivity of well over 100. Both experimental reports and molecular dynamic simulations[3] show the promise of this material. While it is possible to create poly-

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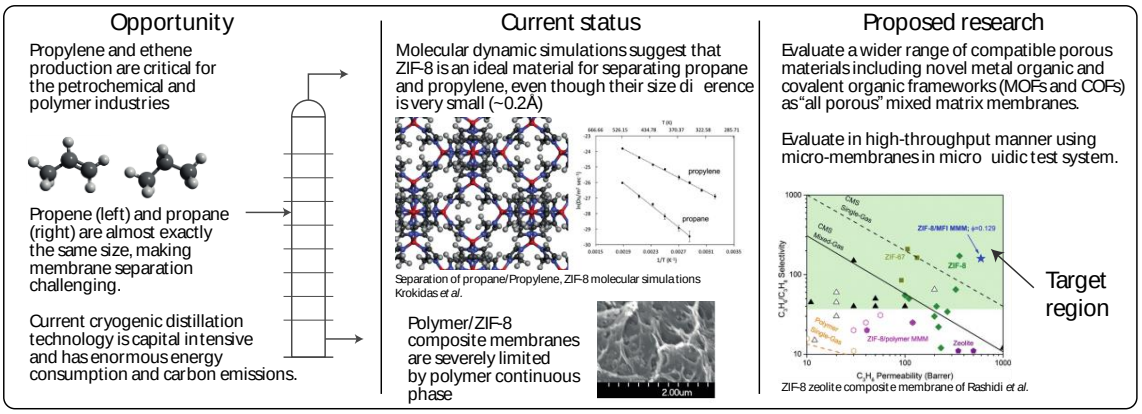
mer/ZIF-8 composite membranes (for example ZIF-8 supported on polymer hollow fibres[4] or in mixed matrix membranes), these generally offer only marginal improvement over polymer membranes, far below the potential of ZIF-8 and indeed other emerging nanoporous materials (such as covalent organic frameworks, COFs).



Proposed research

A breakthrough in exploiting the true potential of high-performance materials like ZIF-8 has been published recently, showing that pure nanoporous mixed matrix materials comprised of a MOF dispersed in a continuous zeolite phase, can achieve separation factors with excellent membrane permeance[5]. This project will explore multiple new combinations of mixed-matrix membranes using this new "all porous" philosophy, in particular exploring the potential for other newly discovered MOF and COF materials. The research will be largely experimental at KIT, with a focus on materials synthesis, characterisation and formation into millimetre-size membranes for performance testing in compact, robust micro-membrane test devices. This leverages the unique expertise of the Institute for Micro Process Technology in designing and constructing advanced microfluidic devices, to allow for high-throughput materials development with small membrane samples. Simultaneously, the Chinese collaborator will develop fundamental computer models (i.e. molecular dynamic simulations) and macro scale models (i.e. process engineering models), validated with the experimental data, and guiding the materials discovery towards promising new materials, while also driving towards industrially relevant membrane properties. This will allow for both research partners (KIT and the Chinese Partner) to be actively involved in the collaboration from the beginning, with experimental and computer-based aspects pursued collaboratively and in parallel.

References

[1] D. S. Sholl and R. P. Lively, "Seven chemical separations to change the world," *Nature*, vol. 532, no. 7600, pp. 435–437, 2016.

[2] CEFIC, "Facts & Figures of the European Chemical Industry," 2018.

[3] P. Krokidas, M. Castier, S. Moncho, E. Brothers, and I. G. Economou, "Molecular Simulation Studies of the Diffusion of Methane, Ethane, Propane, and Propylene in ZIF-8," *J. Phys. Chem. C*, vol. 119, no. 48, pp. 27028–27037, 2015.

[4] M. J. Lee, M. R. Abdul Hamid, J. Lee, J. S. Kim, Y. M. Lee, and H.-K. Jeong, "Ultrathin

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zeolitic-imidazolate framework ZIF-8 membranes on polymeric hollow fibers for propylene/propane separation," *J. Memb. Sci.*, vol. 559, pp. 28–34, 2018.

[5] F. Rashidi, J. Leisen, S.-J. Kim, A. A. Rownaghi, C. W. Jones, and S. Nair, "All-Nanoporous Hybrid Membranes: Redefining Upper Limits on Molecular Separation Properties," *Angew. Chemie - Int. Ed.*, vol. 58, no. 1, pp. 236–239, 2019.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

The Chinese Collaboration Partner Institute should have complementary research expertise to that of the Helmholtz Institution. In this case, the Institute at KIT has strong materials synthesis, characterisation and device development expertise. It would be highly advantageous if the Chinese Collaboration Partner had excellent capabilities in the simulation of gas transport in complex porous materials, as well as process simulation expertise.

Note: at present, a partner is sought.

Required qualification of the post-doc:

- PhD in Chemical Engineering, Materials Science, Materials Chemistry
- Experience with synthesis of porous materials, materials characterisation
- Additional skills in preparation and testing of polymer or inorganic or composite membranes for gas separation would be an advantage.

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team

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