Editorial

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Diffusion in nanoporous solids, i.e. the irregular movement of guest molecules in a nanoporous host material, is among the most important fundamental phenomena in nature. It arises as a consequence of the randomness of the interactions between the components involved, making it a fascinating topic for basic research. Furthermore, diffusion often determines the performance of these materials in technological applications for upgrading matter by mass separation or chemical conversion, since the gain in value-added products can never be faster than allowed by the rate of mass transfer.

In the middle of the last century zeolites were introduced for industrial scale mass separation and shape-selective catalysis, leading to a substantial increase in productivity. It was widely assumed that the mass transfer rate in such processes was controlled by the rate of guest diffusion in the interior of the host crystals. It thus came as a great surprise when, for several host–guest systems, the intra-crystalline diffusivities were found by direct measurement to notably exceed the values estimated from the rate of molecular uptake and release, suggesting the existence of additional transport resistances. Mass transfer in zeolites and, more generally, in nanoporous materials was thus recognized as a more complex phenomenon.

The direct measurement of intra-crystalline diffusion became possible through the application of the pulsed field gradient (PFG) technique of NMR, established by one of us (JK) as part of his PhD dissertation, under the supervision of Professor Harry Pfeifer, at Leipzig University. Leipzig's connection with NMR dates back to Felix Bloch, one of the discoverers of NMR (and Nobel Prize winner for Physics in 1952), who (with Werner Heisenberg as his mentor) defended his PhD work in Leipzig.

The advent of PFG NMR in zeolite science and technology in the seventies of the last century falls into a time when the world was still divided by the Iron Curtain. Richard Ernst, Nobel Prize winner for Chemistry in 1991 for developing “high-resolution” NMR, alluded to this when, during a lecture in Leipzig in 1992, he recognized Leipzig as the “East Pole” of Nuclear Magnetic Resonance. Although the Iron Curtain notably impeded scientific exchange, it did not completely exclude it. Owing to their involvement in the research program of the Academies of Sciences of the Eastern countries and their cooperation with colleagues in Berlin (Wolfgang Schirmer, Martin Bülow, Jürgen Caro), Prague (Milan Kocirik, Arlette Zikanova), Moscow (Michail Dubinin, Albert Voloshchuk) and Leningrad (Sergey Zhdanov), researchers in Leipzig also made contact with their colleagues on the other side of the Iron Curtain. The textbook “Diffusion in Zeolites” (Wiley, 1992) authored by two of us (JK and DMR) emerged from these contacts and illustrates their fertility. With so far more than 2500 references in Google Scholar, this has become a standard reference in the field.

These contacts intensified with the breakdown of the Iron Curtain, benefitting from the emerging research programmes. It was, in particular, the cooperation between representatives of the different techniques of diffusion measurement that received generous support, notably from the German Science Foundation in re-united Germany and from its partner organizations all over the world and by the European Commission.

Our special gratitude for generous support goes to the Alexander von Humboldt Foundation. RV came as a Humboldt fellow to Leipzig and the presentations of the Max Planck Research Award to DMR and JK in 1993 and of the Humboldt Research Award to DMR in 2002 have most significantly fostered our collaboration, leading to a follow up of our book on diffusion in zeolites in 2012, now under the more general title “Diffusion in Nanoporous Materials” with Doros Theodorou as a co-author.

Research within the thus established networks attempted to achieve the greatest possible coherence in the messages

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resulting from the application of different techniques for diffusion measurement. Attainment of such coherence, however, turned out to be quite complicated since the conditions for the application of different measurement techniques are often different from each other and, sometimes, mutually exclusive. Similar complications are known also from other fields of research and we benefitted greatly from the advice provided by Matthias Thommes based on his experience with the updating of an IUPAC (International Union of Pure and Applied Chemistry) Technical Report on “Physisorption of Gases, with Special Reference to the Evaluation of Surface Area and Pore Size Distribution”. Thus, during one of DMR’s visits in Leipzig, there emerged, among the three of us, the idea to launch a similar activity within the field of diffusion, with the intention “to provide a first comprehensive set of guidelines for measurements and reporting of the diffusion properties of chemical compounds in nanoporous materials serving for catalytic, mass separation and other relevant purposes.”

Our cordial thanks go to Stefano Brandani, Marc-Olivier Coppens, Shamsuzzaman Farooq, Herve Jobic, Douglas LeVan, William Price, Peter I. Ravikovitch and Alexander Stepanov for their consent and support in contacting IUPAC with the suggestion to establish a Task Group dedicated to this mission—and to IUPAC itself for, eventually, approving and supporting this initiative (https://iupac.org/projects/project-details/?project_nr=2015-002-2-100).

As a first step towards providing “a set of guidelines”, the present Thematic Issue of the Adsorption Journal collects research work considering “Diffusion in Nanoporous Solids” from quite different perspectives. This includes, in particular, the presentation of the different options for experimental measurement emphasizing their potential, limitations and hidden pitfalls. Treatises on theory and molecular modelling are also included. They are intended to support data interpretation and, equally importantly, to prevent data misinterpretation. We also wanted to avoid a one-sided approach, as is sometimes found in modelling work, when no reference is made to real experiments.

For the future, the task remains to condense and supplement the statements in this collection of articles so that the intended “guidelines for measurements and reporting of the diffusion properties ...” can indeed emerge from them. All contributors to this Thematic Issue, just as we ourselves, are therefore keen to receive comments and feedback from readers.

Upcoming conferences in the field, notably including the “International Zeolite Conferences” and the conference series on “Fundamentals of Adsorption”, will provide ideal forums for the exchange of ideas. In this context, the “Diffusion Fundamentals” conference series has a special significance. This conference series, which was initiated in Leipzig in 2005, deals with the random movement of objects

(both physical and non-physical) in general. Diffusion in nanoporous materials has always been among the topics covered. Among the local organizers there have been Stefano Brandani (L’Aquila, 2007), Doros Theodorou (Athens, 2009), Marc-Olivier Coppens (Troy, N.Y. 2011), Jürgen Caro (Dresden, 2015) and Andreas Fröba (Erlangen, 2019). We are much obliged to them as well as to Rafal Abdank-Kozubski who will continue this tradition during the upcoming 9th Diffusion-Fundamentals Conference in September 2022 in Krakow. He has agreed to provide us with the opportunity to organize, within the framework of the conference, a workshop specifically dedicated to discussing the issues emerging from this Thematic Issue. The aim of this workshop will be to refine our recommendations concerning diffusion measurements and prepare the basis for the formal “guidelines” that the IUPAC diffusion task group is expected to deliver. Since 2015, the Diffusion-Fundamentals Conferences have been organized under the auspices of the Saxon Academy of Sciences and Humanities, which brings us back to Werner Heisenberg, who once served as the secretary of its Mathematical-Natural Sciences Class.

In conclusion, we would like to express our gratitude to all authors and reviewers who have contributed to this issue, notably including Shamsuzzaman Farooq (former Editor of Adsorption) for the invitation to use, for this purpose, the option of a Thematic Issue of the Adsorption Journal, and Stefano Brandani, the present Editor-in-Chief of Adsorption, jointly with Shalini Arivazhagan, Annushrie Arravind, Davide Migliorini, Karthikeyan Sekaran, and Katie Tunkavige, for their cordial guidance during establishment of this Thematic Issue. We hope that this issue will stimulate your kind interest and, jointly with all authors, we look forward to receiving your feedback.

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