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MOF sensors for contaminant capture and detection: cooperative computational-experimental screening approach

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The remarkable mastery over chemical synthesis in the modern world has drastically enriched humanity. At the same time, our activity often results in significant emissions of undesirable contaminants, including toxic gases (NOx, SOx, CO), volatile organic compounds (BTEX, esters, aldehydes, ⋯) alongside other volatile compounds posing threats to both human health and sensitive machinery. Therefore, the detection and abatement of airborne contaminants at low levels (ppb to ppm) is an ongoing challenge for maintaining a clean and safe environment, particularly in regulated spaces, such as clean rooms, satellites, and indoor living spaces.

In this context, framework materials like MOFs and COFs appear as promising materials due their tailorable chemical and physical properties and highly porous structures, acting as sorption media for direct air capture of contaminants,[1] or as components in electronic devices designed for monitoring their concentration.[2] Nevertheless, given the large number of synthesizable frameworks [3] the choice of a material to target a specific contaminant is more often than not a question of serendipity.[4]

To overcome this problem, a generalized approach is herein given for screening MOFs for specific contaminant molecules. This method combines high-throughput molecular simulations to highlight key promising materials, followed by advanced adsorption experiments at very low contaminant concentrations and sensing. We further detail several classes of MOF materials which were identified through this approach that are applicable to the capture and detection of common contaminants in the space industry (i) siloxanes, (ii) aromatics and (iii) esters.

Participation

In-Person

References

[1] C. Lai, Z. Wang, L. Qin, Y. Fu, B. Li, M. Zhang, S. Liu, L. Li, H. Yi, X. Liu, X. Zhou, N. An, Z. An, X. Shi, C. Feng, Coordination Chemistry Reviews 2021, 427, 213565.
[2] M. D. Allendorf, R. Dong, X. Feng, S. Kaskel, D. Matoga, V. Stavila, Chem. Rev. 2020, 120, 8581–8640.
[3] P. Z. Moghadam, A. Li, X.-W. Liu, R. Bueno-Perez, S.-D. Wang, S. B. Wiggin, P. A. Wood, D. Fairen-Jimenez, Chem. Sci. 2020, 11, 8373–8387.
[4] S. Curtarolo, G. L. W. Hart, M. B. Nardelli, N. Mingo, S. Sanvito, O. Levy, Nature Mater 2013, 12, 191–201.

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