

Special section – Crystallography and properties of metal–organic framework (MOF) compounds

Metal–organic frameworks (MOFs) are known for their wide range of potential applications, including gas sorption, gas storage, gas separation, catalysis, sensors, drug delivery, imaging, electronic devices, and environmental sustainability, yet our fundamental understanding of the properties of MOF materials is incomplete. As functional MOF materials are envisioned to play an important role in our modern society and in future economic and social progress, the underlying crystallographic information for these materials is of great importance for many research communities.

The goal of the special sections has been to focus on the latest developments in the cross-disciplinary fields of structure science and MOF materials. The papers have been published throughout the four 2019 issues and the March 2020 issue of *Powder Diffraction*. Progress in measurement capabilities with *in situ*, *in operando*, multi-modal, and high-pressure crystallographic techniques are addressed in these journal sections. The types of materials covered include bulk powders, single crystals, amorphous solids, thin films, and nanostructures. The special sections encompass up-to-date MOF research topics as well as reviews that present new evaluations and analyses of the published work. The present issue consists of the last invited paper of the special sections; it is entitled “Crystal Structure of 1-propanethiol-Co₂(dobdc) from Laboratory X-ray Powder Diffraction Data” by Professor Tomce Runcevski *et al.* of Southern Methodist University.

In summary, the list of manuscripts that have been published in the past four issues and the current issue of *Powder Diffraction* are:

1. Parise, J. B., Chen, X., Plonka, A. M., Woerner, W. R., Banerjee, D., Connors, D., and Goroff, N. (2019). “XRD-DSC: a screening tool for identifying effective MOFs for selective gas sorption from humid gas streams,” *Powd. Diffr.* 34, 3–12.
2. Lawson, M., Horn, J., Wong-Ng, W., Espinal, L., Lapidus, S. H., Giang Nguyen, H., Meng, Y., Suib, S. L., Kaduk, J. A., and Li, L. (2019). “First-principles study of carbon capture and storage properties of porous MnO₂ octahedral molecular sieve OMS-5,” *Powd. Diffr.* 34, 13–20.
3. Sornadurai, D., Sarguna, R. M., and Sridharan, V. (2019). “Variation of structural parameters in dimethylammonium manganese formate [(CH₃)₂NH₂]Mn(HCOO)₃ by substitution of transition metals (M=Zn, Co and Ni): by powder XRD method,” *Powd. Diffr.* 34, 124–129.
4. Barreda, O., Lorzing, G. R., and Bloch, E. D. (2019). “Mechanochemical synthesis of two-dimensional metal–organic frameworks,” *Powd. Diffr.* 34, 119–123.
5. Wong-Ng, W., Nguyen, H. G., Espinal, L., Siderius, D. W., and Kaduk, J. A. (2019). “Powder X-ray structural and reference diffraction patterns for three forms of porous aluminum terephthalate, MIL-53(AL),” *Powd. Diffr.* 34, 216–226.
6. Cockayne, E. (2019). “Density functional theory meta GGA study of water adsorption in MIL-53(Cr),” *Powd. Diffr.* 34, 227–232.
7. Sun, H. and Wu, D. (2019). “Recent advances in experimental thermodynamics of metal–organic frameworks,” *Powd. Diffr.* 34, 297–301.
8. Cook, L. P., Brewer, G. A., Siderius, D., and Wong-Ng, W. (2019). “Topology of voids and channels in selected porphyrinic compounds,” *Powd. Diffr.* 34, 302–310.
9. Leften, J. B., Pekor, K.B., Sethio, D., Kraka, F., and Runcevski, T. (2020). “Crystal structure of 1-propanethiol-Co₂(dobdc) from laboratory X-ray powder diffraction data” *Powd. Diffr.* 35 (this issue).

The guest editors anticipate that these papers will serve the community as the reference for modern measurement capabilities, data analysis, and materials insight.

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