Oral presentation

Analysis of MOFs underlying nets with ToposPro: occurrences and entanglements

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ToposPro[1] since 2014 has been used by many MOFs chemists around the world to deconstruct MOFs into underlying nets [2]. Accurate data about MOFs topologies is the base for machine-assisted search for complex reticular correlations and design of new functional materials. We will introduce latest tools that include the database of underlying nets TTD (accessible via TopCryst) [3], the analysis of rod MOFs [4] and the topological approach based on the concept of Extended Ring Nets (ERNs) [5] that allows to characterize any entanglement to the greatest detail ever achieved.

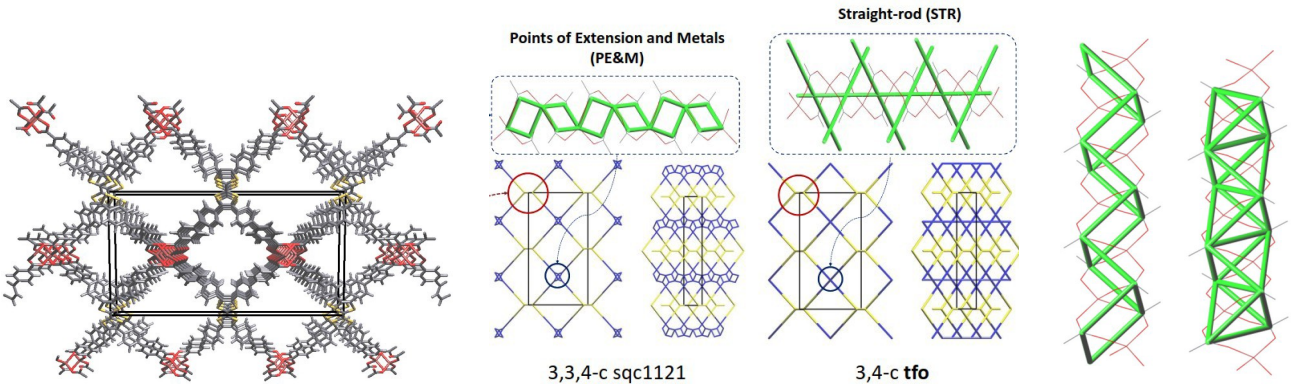

Figure 1. Analysis of the possible underlying nets for a rod-MOF Zn_2TTFTB [6]: which is best? Which is useful?

[1] *Applied Topological Analysis of Crystal Structures with the Program Package ToposPro* Blatov, V.A., Shevchenko, A.P. & Proserpio D.M. (2014). *Cryst. Growth Des.*, **14**, 3576-3586. https://topospro.com/ http://update.topospro.com/statistics/

[2] *Deconstruction of Crystalline Networks into Underlying Nets: Relevance for Terminology Guidelines and Crystallographic Databases,* Bonneau, C., O'Keeffe, M., Proserpio, D.M., Blatov, V.A., Batten, S.R., Bourne, S.A., Lah, M.S., Eon, J.-G., Hyde, S.T., Wiggin, S.B. & Öhrström, L. (2018). *Cryst. Growth Des.*, **18**, 3411-3418.

[3] *Topological representations of crystal structures: generation, analysis and implementation in the TopCryst system.* Shevchenko, A.P. Shabalin, A.A., Karpukhin, I.Y. & Blatov, V.A. (2022). *Sci. Technol. Adv. Mater.: Methods*, **2**, 250-265. https://topcryst.com

[4] *Diverse π–π stacking motifs modulate electrical conductivity in tetrathiafulvalene-based metal–organic frameworks.* Xie, L.S., Alexandrov, E.V., Skorupskii, G., Proserpio, D.M. & Dincă, M. (2019) *Chem. Sci.*, **10**, 8558-8565.

[5] *How 2-periodic coordination networks are interweaved: entanglement isomerism and polymorphism.* Alexandrov, E.V., Blatov, V.A. & Proserpio, D.M. (2017). *CrystEngComm*, **19**, 1993-2206.

[6] *A redox active rod coordination polymer from tetrakis(4-carboxylic acid biphenyl) tetrathiafulvalene.* Zigon, N., Solano, F., Auban-Senzier, P., Grolleau, S., Devic, T., Zolotarev, P.N., Proserpio, D.M., Barszcz, B., Olejniczak, I. & Avarvari N. (2024). *Dalton Trans.*, **53**, 4805–4813.

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