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Investigating negative thermal expansion in aliphatic metal-organic frameworks

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Negative thermal expansion (NTE) involves the unconventional behaviour of material contraction upon heating and has been observed in some metal organic frameworks (MOFs). Investigations into the mechanism governing NTE are highly important for practical applications for when it is undesirable for materials to expand upon heating. Previous investigations focused on aromatic and single component frameworks, our goal is to expand into the realm of aliphatic linkers such as cubane-1,4-dicarboxylate (1,4-cdc) and bicyclo[1.1.1]pentane-1,3-dicarboxylate (1,3-pdc), which may introduce unencountered dynamic motions.[1]

Single-component aliphatic MOFs, 3DL-MOF-1 ([Zn4O(1,3-pdc)3]) and CUB-5 ([Zn4O(1,4-cdc)3]) were explored using powder diffraction (PD) techniques.[2] The aliphatic MOFs demonstrated enhanced NTE, in comparison to its aromatic MOF-5 analogue . Investigations on the host-guest effects on NTE behaviour[3] were explored using neutron PD at the ACNS by charging 3DL-MOF-1 with CO2 guest molecules. Successful NTE quenching was achieved at higher CO2 loading.

To extend our understanding of aliphatic influences on NTE behaviour, we study a series of moisture stable multicomponent frameworks.[4] Using synchrotron PD and single crystal X-ray diffraction we investigate the NTE behaviour of quaternary MOFs (three linkers and one node) by varying the aliphatic linker in each system. We hope to identify the key characteristics of aliphatic linkers that dictates NTE behaviour.

[1] J. Perego et al., Nature Chemistry 2020, 12, 845.
[2] L. K. Macreadie et al., ACS Applied Materials & Interfaces 2021, 13, 30885.
[3] J. E. Auckett et al., Nature communications 2018, 9, 1.
[4] L. K. Macreadie, et al., Angewandte Chemie International Edition 2020, 59, 6090.

Level of Expertise

Student

Presenter Gender

Woman

Pronouns

She/Her

Which facility did you use for your research

Australian Centre for Neutron Scattering

Students Only - Are you interested in AINSE student funding

Yes

Do you wish to take part in the Student Poster Slam

Yes

Condition of submission

Yes

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