Electronic Supplementary Material (ESI) for Chemical Communications

Postsynthetic modification of epitaxially grown, highly oriented MOF thin films.

Osama Shekhah,*[a] Hasan K. Arslan,[a] Kun Chen,[b] Michael Schmittel,[b] Robert Maul,[c] Wolfgang Wenzel[d] and Christof Wöll[a]

[a] *Institut für Funktionelle Grenzflächen (IFG), Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany. Fax: +49-721-60823478; Tel: +49-721-608-26946; E-mail: osama.shekhah@kit.edu*
[b] *Organische Chemie 1, Department Chemie und Biologie, Universität Siegen, Siegen, Germany. Fax: +49-271-7403270; Tel: +49-271-7404356; E-mail: schmittel@chemie.uni-siegen.de*
[c] *Steinbuch Center for Computing, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany and DFG Center for Functional Nanostructures, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany, Fax: +49-721-60826386; Tel: +49-721-608-28901; E-mail: robert.maul@kit.edu*
[d] *Institut für Nanotechnology (INT), Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany. Fax: +49-721-60826386; Tel: +49-721-608-28901; E-mail: wolfgang.wenzel@kit.edu*

Electronic Supplementary Information

Fig. S1. IRRAS data of a $[Cu_2(NH_2\text{-bdc})_2(dabco)]$ SURMOF grown on a MUD SAM.

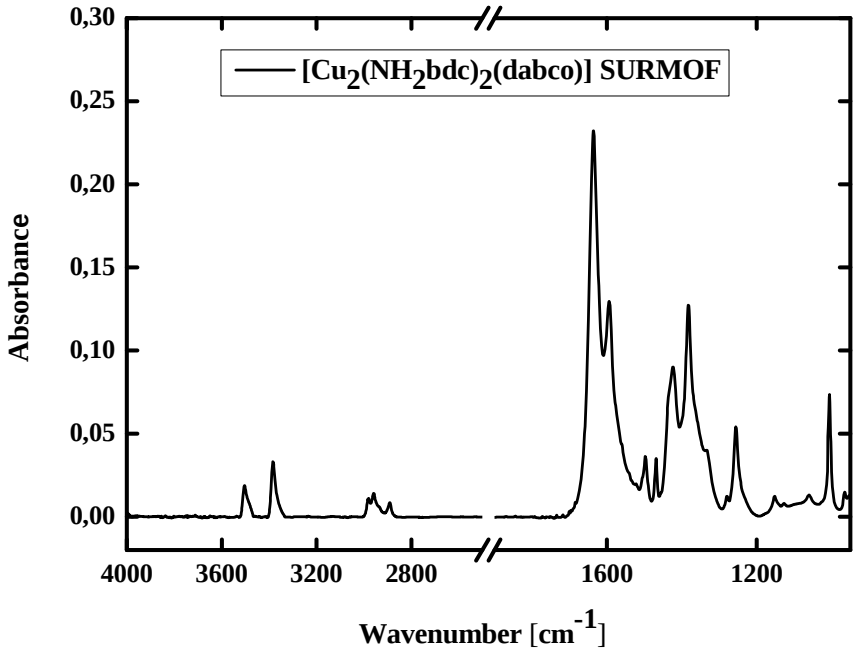
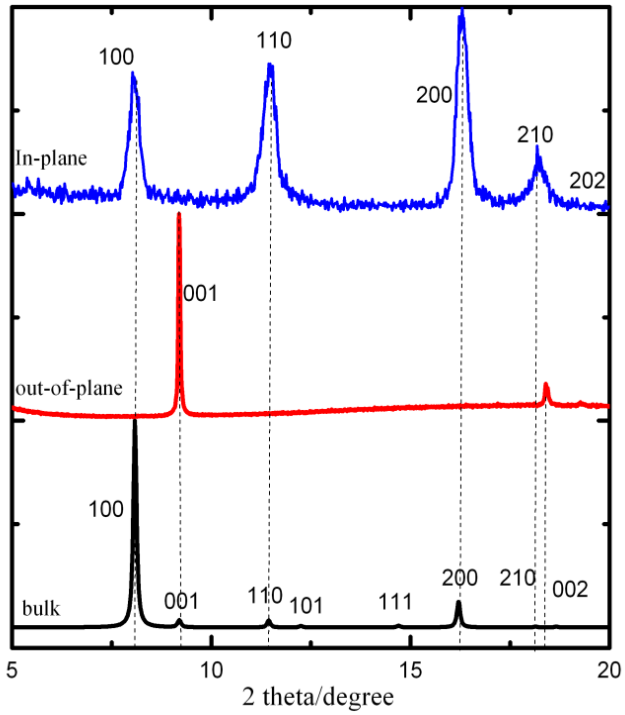


Fig. S2. XRD data for a $[Cu_2(NH_2\text{-bdc})_2(dabco)]$ MOF bulk (black), out-of-plane (red) and in-plane (blue), grown on a MUD SAM.



Scheme S1. Schematic representation of postsynthetic modification where a synthon is attached to a MOF lattice, e.g. by using an amino-isocyanate coupling reaction.

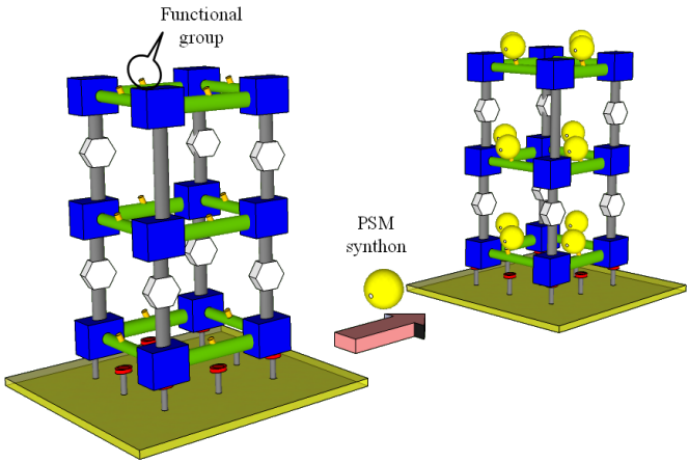


Fig. S3. Comparison of IRRAS from as-synthesized [$Cu_2(NH_2\text{-bdc})_2$(dabco)] SURMOF (black), prepared by the LPE method and $Cu_2(NH_2\text{-bdc})_2$(dabco)] SURMOF modified with n-butylisocyanate (red).

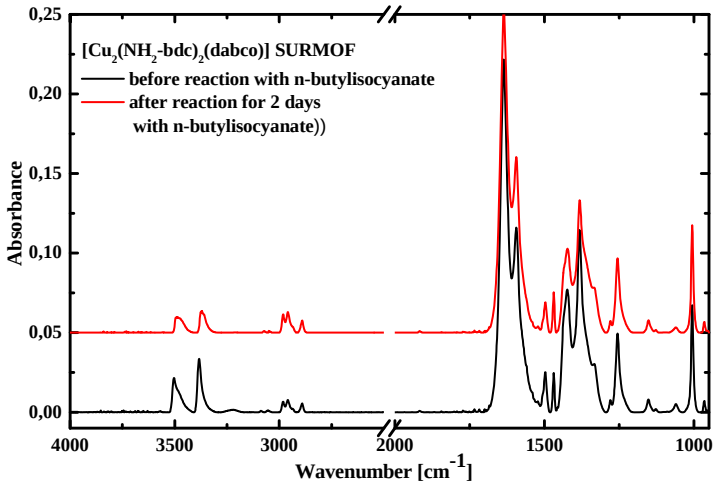


Fig. S4 Comparison of IR data from an as-synthesized [Cu2(NH2-bdc)2(dabco)] SURMOF (black) prepared by the LPE method and a [Cu2(NH2-bdc)2(dabco)] SURMOF modified with 4-fluorophenylisothiocyanate (blue) and modified with 1-ferrocenylmethylisocyanate (red).

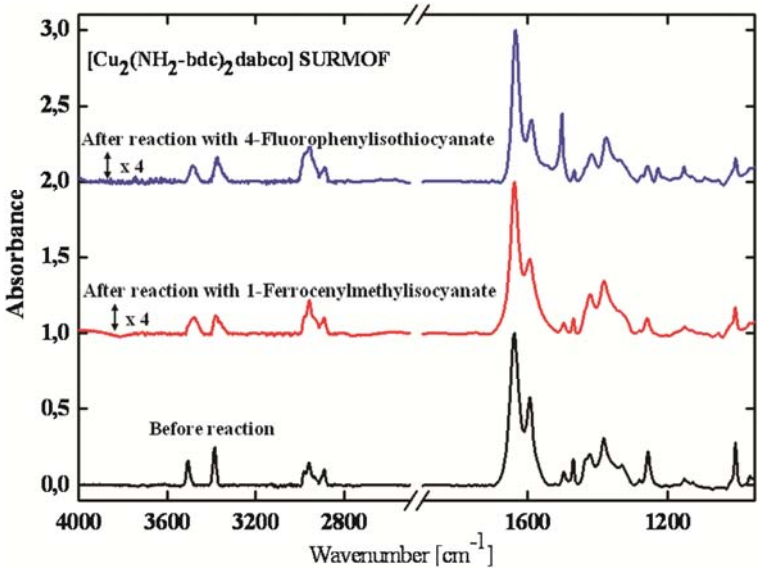


Fig. S5. Comparison of XRD patterns from as-synthesized [$Cu_2(NH_2\text{-bdc})_2(dabco)$] (black), prepared by the lbl method. $Cu_2(NH_2\text{-bdc})_2(dabco)$] modified with n-butylisocynate (red).

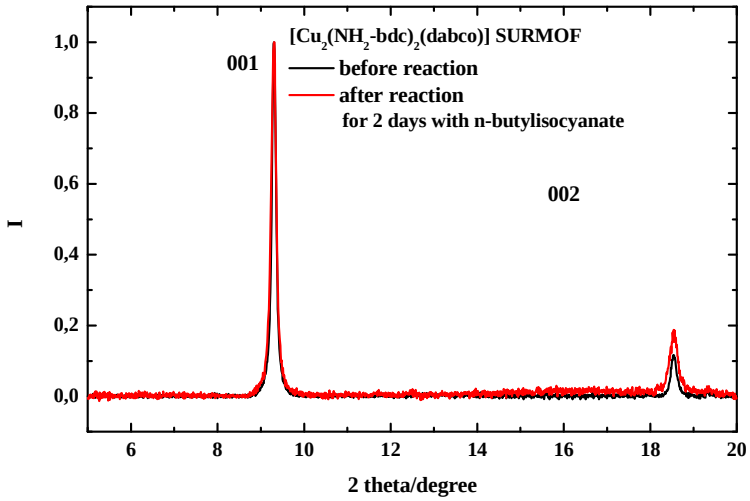
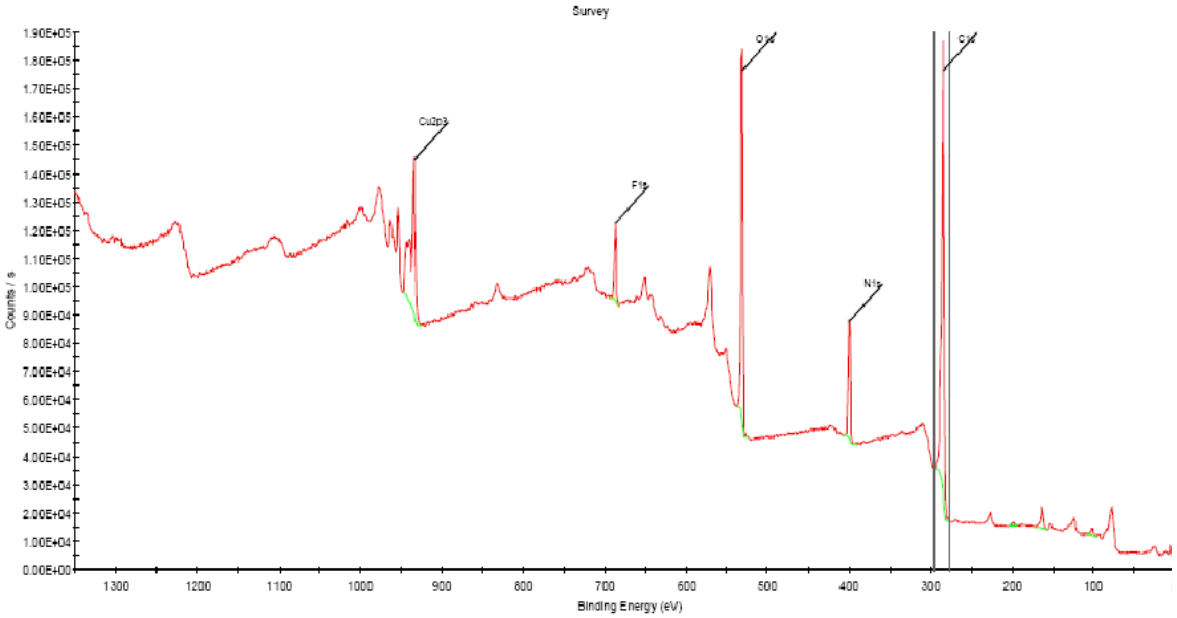


Fig. S6. XP spectra $[Cu_2(NH_2\text{-bdc})_2(dabco)]$ modified with 4-fluorophenyl-isothiocyanate (top) and 1-ferrocenylmethylisocyanate (bottom).



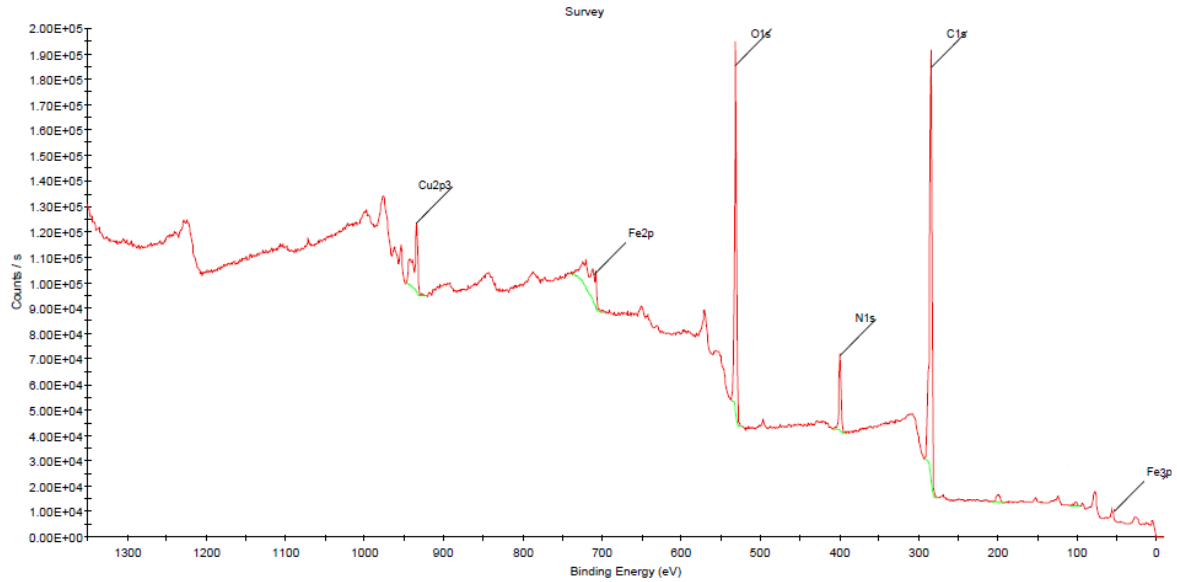


Fig. S7. Geometry of a [Cu_2(NH_2-bdc)(dabco)] MOF after covalently attaching three 4-fluorophenyl-isothiocyanate -units (green) per pore, as obtained from MD-simulations. The grey surface indicates the free space in the unit cell of the empty MOF before the PSM process.