Electronic Supplementary Material (ESI) for CrystEngComm.

An approach for the pore-centred description of adsorption in hierarchical porous materials

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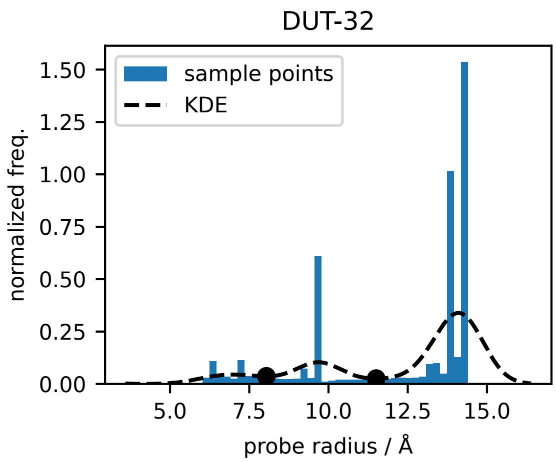
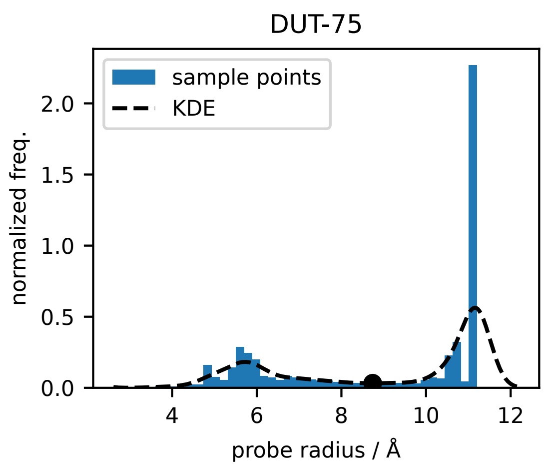
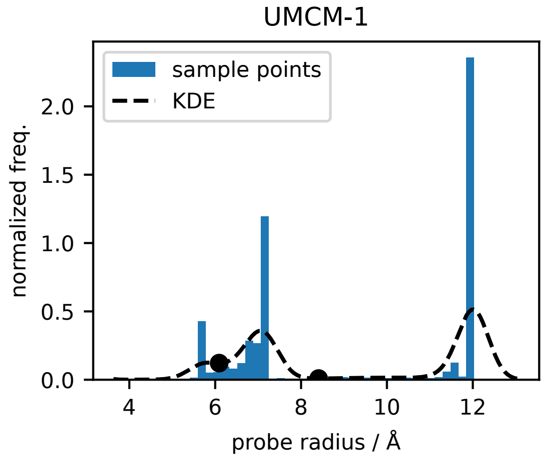


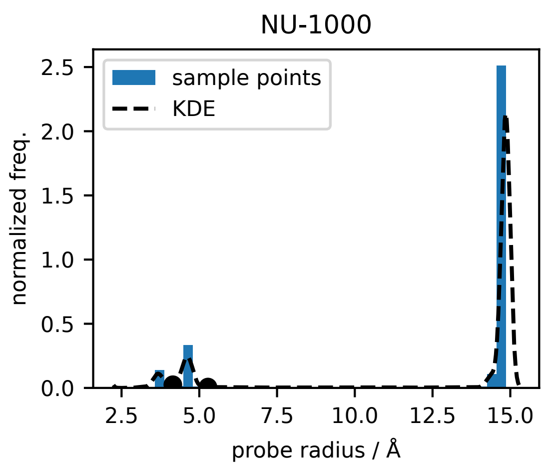
Supplementary Figure 1: Kernel destiny estimation (KDE) of the pore size distribution compared to the pore size histogram for DUT-32. Minimum points (black points) depict the identified pore limits.



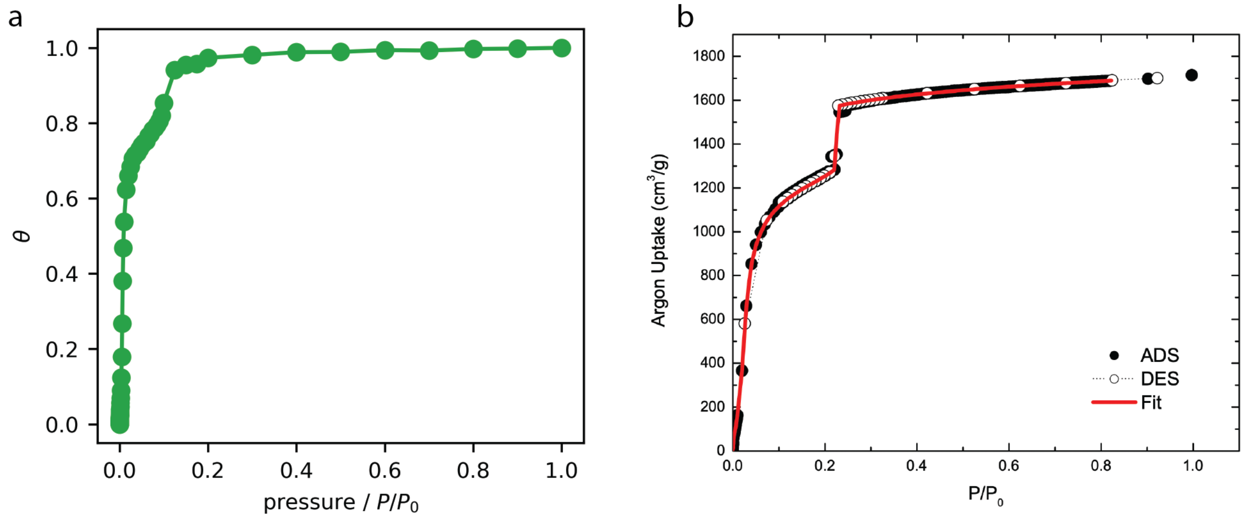
Supplementary Figure 2: Kernel destiny estimation (KDE) of the pore size distribution compared to the pore size histogram for DUT-75. Minimum points (black points) depict the identified pore limits.



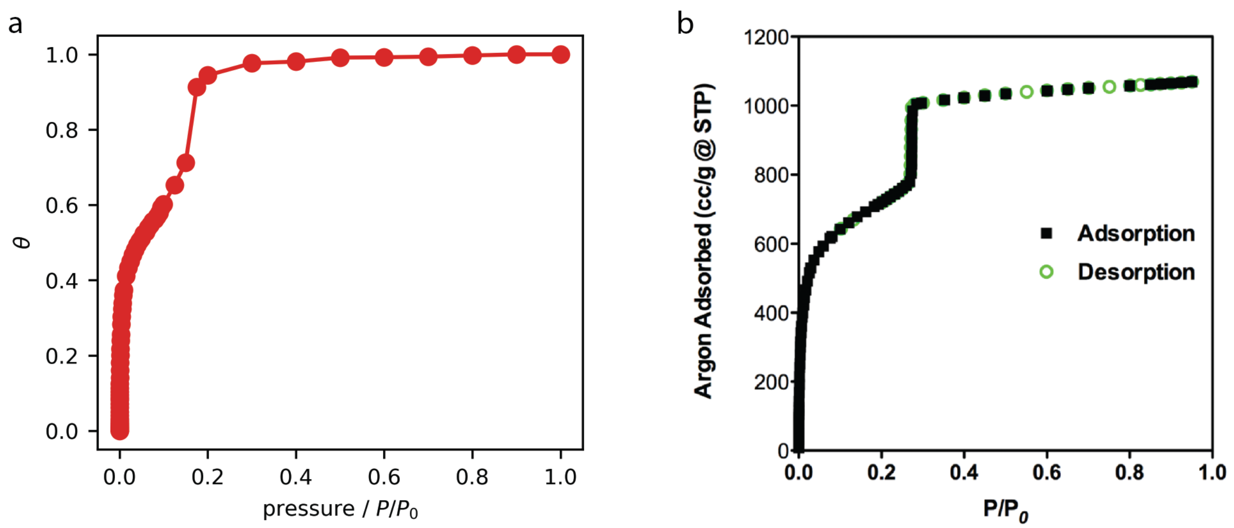
Supplementary Figure 3: Kernel destiny estimation (KDE) of the pore size distribution compared to the pore size histogram for UMCM-1. Minimum points (black points) depict the identified pore limits.



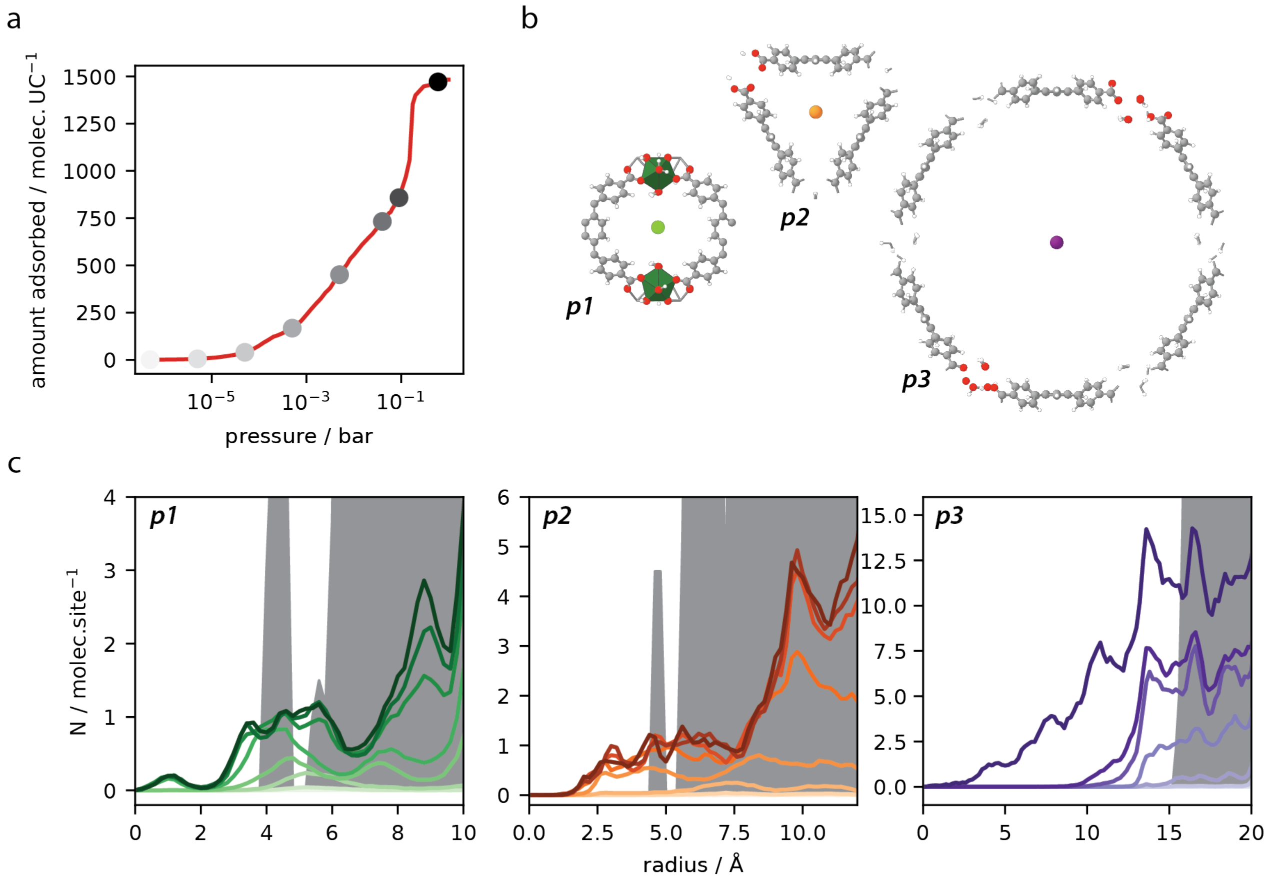
Supplementary Figure 4: Kernel destiny estimation (KDE) of the pore size distribution compared to the pore size histogram for NU-1000. Minimum points (black points) depict the identified pore limits.



Supplementary Figure 5: Simulated Ar adsorption isotherm of UMCM-1 at 87 K displayed as fractional coverage, θ ((**a**). Experimental Ar adsorption isotherm of UMCM-1 at 87 K reproduced from Ref 1 (**b**).



Supplementary Figure 6: Simulated Ar adsorption isotherm of NU-1000 at 87 K displayed as fractional coverage, θ ((**a**). Experimental Ar adsorption isotherm of NU-1000 at 87 K reproduced from Ref 2 (**b**).



Supplementary Figure 7: Pore-centred view of adsorption in NU-1000. Ar adsorption isotherm at 87 K with the points extracted for radial distribution analysis labelled as points (**a**). Pore environments of the pores found in NU-1000 where the centre of the pore is depicted by a green, orange and purple sphere (**b**). Radial distributions of Ar and framework atoms (grey background) from the centre of each pore for the pressure points labelled in the isotherm (**c**).

References

(1) Koh, K.; Wong-Foy, A.; Matzger, A. *Angewandte Chemie International Edition* **2008**, *47*, 677–680.

(2) Mondloch, J. E.; Bury, W.; Fairen-Jimenez, D.; Kwon, S.; DeMarco, E. J.; Weston, M. H.; Sarjeant, A. A.; Nguyen, S. T.; Stair, P. C.; Snurr, R. Q.; Farha, O. K.; Hupp, J. T. *Journal of the American Chemical Society* **2013**, *135*, 10294–10297.