Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.


# Supporting information

## Promotion of methane storage capacity with metal-organic frameworks of high porosity

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### Additional figures and tables

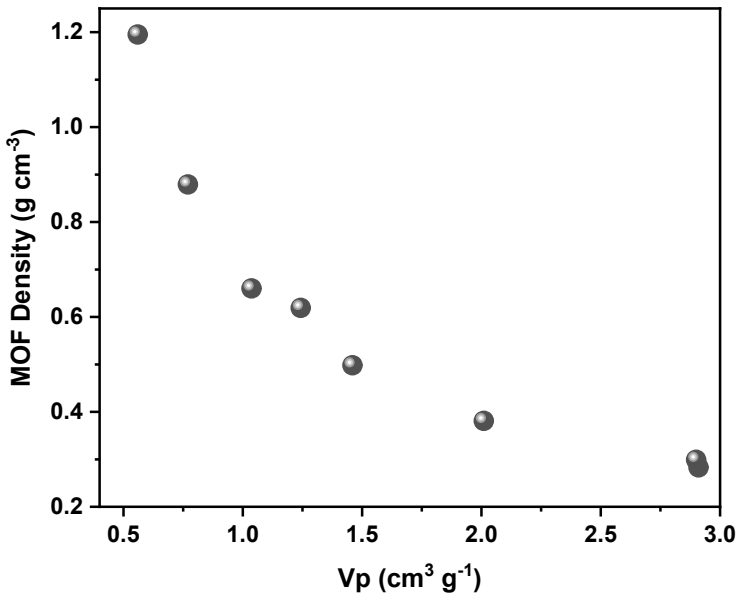


**Figure S1**. MOF density vs pore volume.

**Table S1.** Total adsorption and working capacity at 298 K and 273 K of MOFs discussed

| MOF | Crystal density | Pore volume | Total adsorption 100 bar 298 K | | Total adsorption 100 bar 270 K | | Working capacity 5-100 bar 298 K | | Working capacity 5-100 bar 270 K | | Qst | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $g/cm^3$ | $cm^3/g$ | $cm^3\ cm^{-3}$ | $g\ g^{-1}$ | $cm^3\ cm^{-3}$ | $g\ g^{-1}$ | $cm^3\ cm^{-3}$ | $g\ g^{-1}$ | $cm^3\ cm^{-3}$ | $g\ g^{-1}$ | kJ/mol | |
| Ni-MOF-74 | 1.195 | 0.56 | 281 | 0.17 | 293 | 0.18 | 162 | 0.1 | 135 | 0.08 | 21.4 | 1 |
| HKUST-1 | 0.881 | 0.77 | 277 | 0.23 | 306 | 0.25 | 207 | 0.17 | 195 | 0.16 | 17 | 1 |
| ZJU-105a | 0.66 | 1.037 | 258 | 0.28 | 287 | 0.31 | 203 | 0.22 | 207 | 0.22 | 14.2 | 2 |
| PCN-46a | 0.619 | 1.243 | 260 | 0.30 | 299 | 0.35 | 217 | 0.25 | 235 | 0.27 | 16.6 | 2 |
| NU-1500-Al | 0.498 | 1.46 | 237 | 0.34 | 273 | 0.39 | 202 | 0.29 | 224 | 0.32 | 13.7 | 3 |
| MFU-4l-Li | 0.479 | 1.66 | 248 | 0.37 | 294 | 0.44 | 220 | 0.30 | 251 | 0.38 | 13.3 | 4 |
| BUT-20 | 0.381 | 2.01 | 224 | 0.42 | 260 | 0.49 | 197 | 0.37 | 224 | 0.42 | 12 | 5 |
| NPF-200 | 0.389 | 2.17 | 227 | 0.42 | 275 | 0.51 | 207 | 0.38 | 248 | 0.46 | 10.7 | This work |
| NU-1501-Fe | 0.299 | 2.9 | 218 | 0.52 | 264 | 0.63 | 201 | 0.48 | 239 | 0.57 | 9.6 | 3 |
| NU-1501-Al | 0.283 | 2.91 | 214 | 0.54 | 262 | 0.66 | 198 | 0.5 | 238 | 0.60 | 9.7 | 3 |

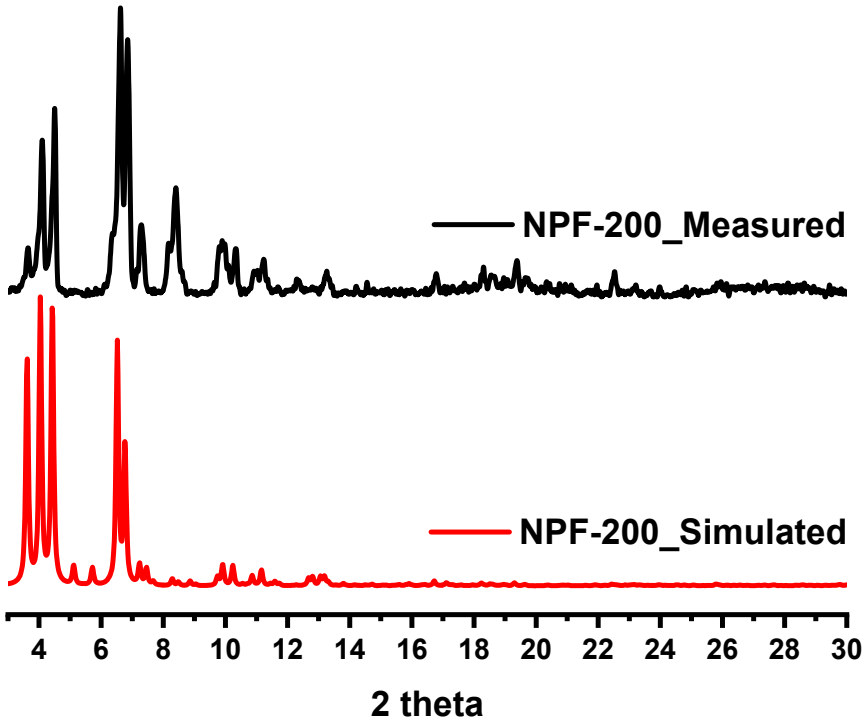


**Figure S2.** PXRD of NPF-200 and comparison with that simulated from single crystal structure.

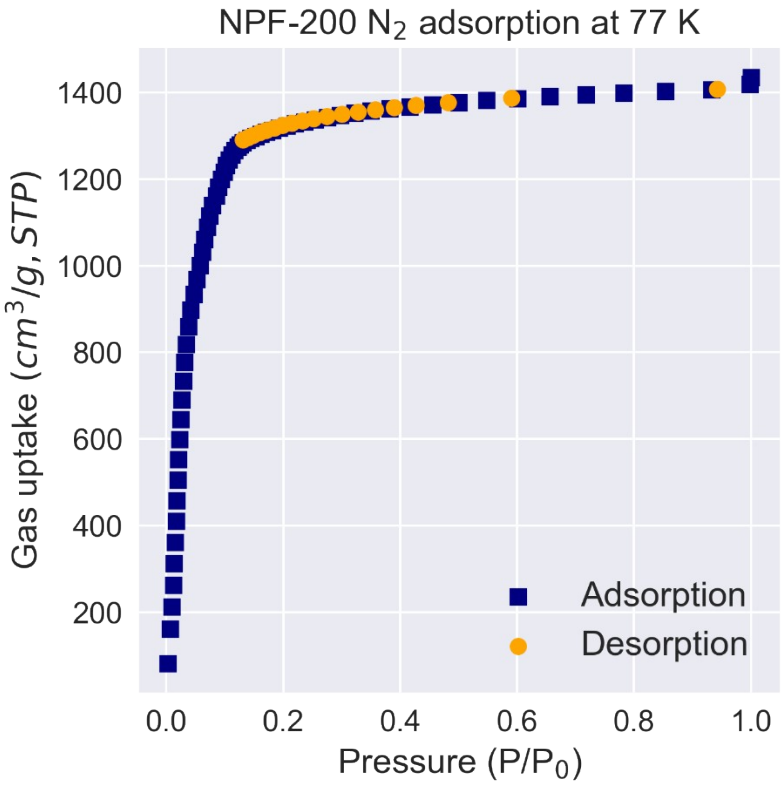


**Figure S3**. $N_2$ adsorption isotherm of NPF-200 at 77 K.

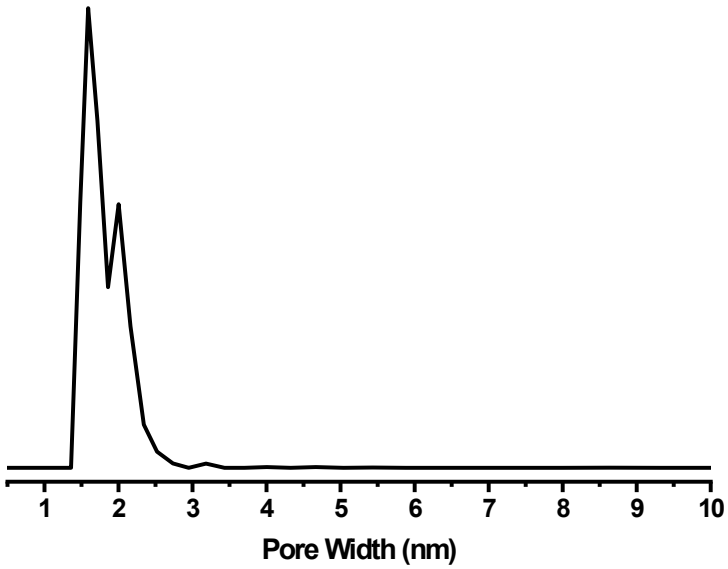


**Figure S4**. Pore size distribution determined from $N_2$ uptake at 77 K.

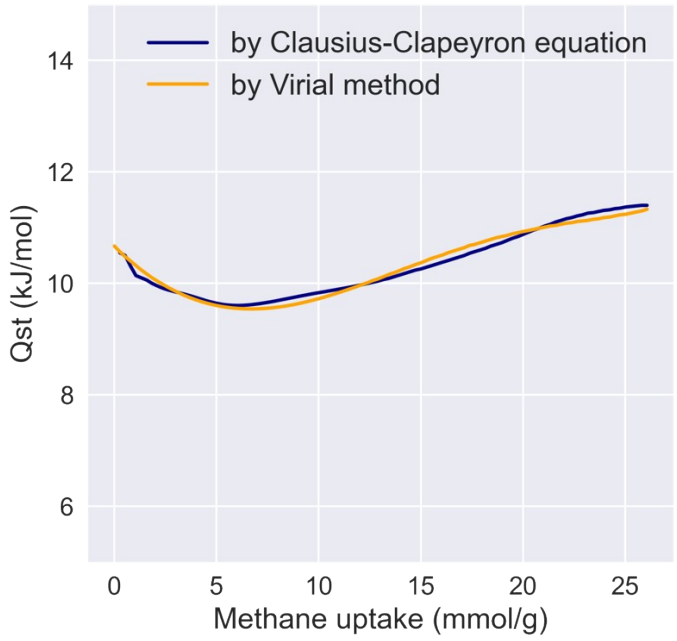


**Figure S5**. Qst of methane adsorption in NPF-200 calculated using virial method.

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**References**


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