Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.
This journal is © The Royal Society of Chemistry 2017

*Supporting Information*

# Ultra-high surface area mesoporous carbons for colossal pre combustion $CO_2$ capture and storage as materials for hydrogen purification

Michael Cox, and Robert Mokaya

School of Chemistry, University of Nottingham, University Park, NG7 2RD Nottingham, UK.

*r.mokaya@nottingham.ac.uk

**Table S1**. Textural properties of polypyrrole-derived activated (PPY-xT) and compactivated (MPPY-4800) carbons compared to other carbons and porous materials that possess varying levels of mesoporosity.

| Sample | Surface area ($m^2$ $g^{-1}$) | Pore volume[a] ($cm^3$ $g^{-1}$) | Mesoporosity[b] (%) | Reference |
|---|---|---|---|---|
| CA-4700 | 3771 | 1.75 (0.21) | 12 | This work |
| AC-0 | 3100 | 1.46 (0.41) | 28 | 1 |
| SU-AC-400 | 4196 | 2.26 (0.70) | 31 | 2 |
| AC-2M | 3420 | 2.22 (0.94) | 42 | 1 |
| UGil-900 | 4200 | 2.41 (n.d.) | | 3 |
| PPY-4700 | 3568 | 2.46 (2.18) | 89 | This work |
| PPY-4800 | 3589 | 2.71 (2.46) | 91 | This work |
| MPPY-4800 | 3934 | 2.92 (2.72) | 93 | This work |
| PPY-5800 | 2974 | 2.85 (2.63) | 92 | This work |
| PPY-3900 | 3285 | 2.60 (2.30) | 88 | This work |
| PPY-4900 | 2842 | 2.77 (2.50) | 90 | This work |
| PPY-5900 | 2798 | 3.54 (3.35) | 95 | This work |
| MOF-210 | 6240 | 3.60 (n.d.) | | 4 |
| NU-100 | 6143 | 2.82 (n.d.) | | 5 |

[a]The values in the parenthesis refer to mesopore volume. [b]Proportion of pore volume arising from mesopores. (n.d. = not determined)

**References**


1. M. Sevilla, W. Sangchoom, N. Balahmar, A. B. Fuertes and R. Mokaya, *ACS Sust. Chem. Eng*., 2016, **4**, 4710.
2. J. He, J. W. F. To, P. C. Psarras, H. Yan, T. Atkinson, R. T. Holmes, D. Nordlund, Z. Bao and J. Wilcox, *Adv. Energy Mater*. 2016, **6**, 1502491.
3. A. S. Jalilov, Y. Li, J. Tian, J. M. Tour, *Adv. Energy Mater*. 2017, **7**, 1600693.
4. H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, J. Kim and O. M. Yaghi, *Science* 2010, **329**, 424.
5. O. K. Farha, A. O. Yazaydın, I. Eryazici, C. D. Malliakas, B. G. Hauser, M. G. Kanatzidis, S. T. Nguyen, R. Q. Snurr and J. T. Hupp, *Nat. Chem*. 2010, **2**, 944.

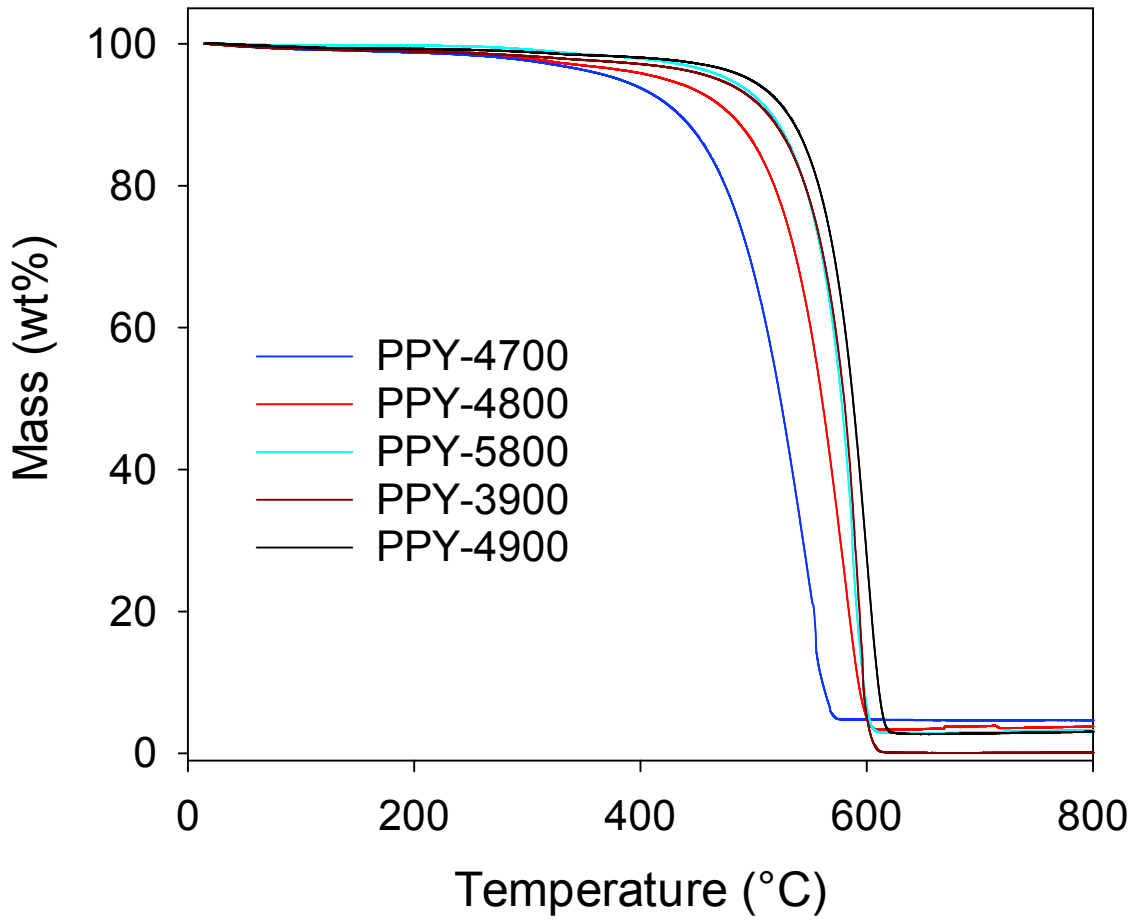
**Table S2**. Total and excess gravimetric $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons and compactivated (MPPY-4800) carbon compared to other carbons and metal organic frameworks (MOFs).

| Sample | $CO_2$ uptake[a] (mmol $g^{-1}$) | | | | | Reference |
|---|---|---|---|---|---|---|
| | 1 bar | 20 bar | 30 bar | 40 bar | 50 bar | |
| CA-4700 | 3.7 | 19.5 (18.0) | 22.3 (19.8) | 24.1 (20.4) | 25.6 (20.5) | This work |
| AC-0 | 2.4 | 20.4 (19.2) | 24.6 (22.5) | 27.1 (24.1) | 28.5 (24.2) | 1 |
| AC-2M | 2.3 | 22.8 (20.7) | 29.2 (26.0) | 34.5 (29.7) | 38.3 (31.7) | 1 |
| SU-AC-400 | 4.3 | 22.4 (20.3) | 28.3 (25.1) | 32.5 (27.5) | 34.9 (28.3) | 2 |
| UGil-900 | 2.6 | 22.9 (21.5) | 29.4 (27.0) | 33.9 (29.6) | 35.2 (30.8) | 3 |
| PPY-4700 | 2.3 | 22.8 (20.6) | 29.6 (26.0) | 35.4 (30.2) | 40.3 (32.9) | This work |
| PPY-4800 | 2.5 | 25.0 (22.5) | 33.0 (29.0) | 39.5 (34.0) | 45.3 (37.2) | This work |
| MPPY-4800 | 2.8 | 28.1 (25.5) | 37.2 (33.0) | 45.6 (39.5) | 54.1 (45.4) | This work |
| PPY-5800 | 1.3 | 24.1 (21.5) | 32.8 (28.7) | 41.8 (35.8) | 50.8 (42.3) | This work |
| PPY-3900 | 2.2 | 23.2 (20.9) | 30.7 (26.9) | 37.5 (32.0) | 44.5 (36.5) | This work |
| PPY-4900 | 2.0 | 23.6 (21.2) | 31.9 (27.9) | 41.4 (34.4) | 49.3 (41.0) | This work |
| PPY-5900 | 2.1 | 25.7 (22.5) | 34.9 (29.7) | 44.6 (37.1) | 55.1 (44.5) | This work |
| MOF-210 | 0.9 | 19.2 (16.0) | 38.9 (33.7) | 55.0 (46.7) | 64.2 (52.5) | 4 |
| NU-100 | 2.7 | 24.6 (22.0) | 40.9 (36.3) | 52.7 (46.8) | | 5 |

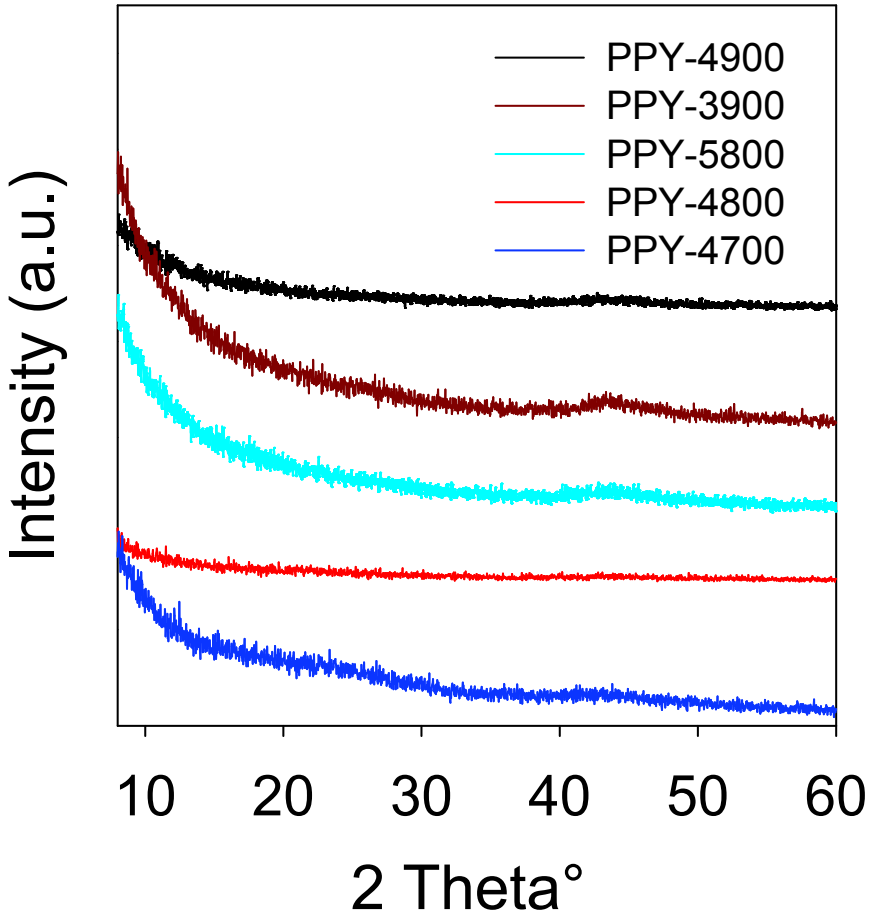
[a]$CO_2$ uptake at 25 $^oC$ and various pressures (i.e., 1, 20, 30, 40 and 50 bar). The values in the parenthesis are excess $CO_2$ uptake.

**References**

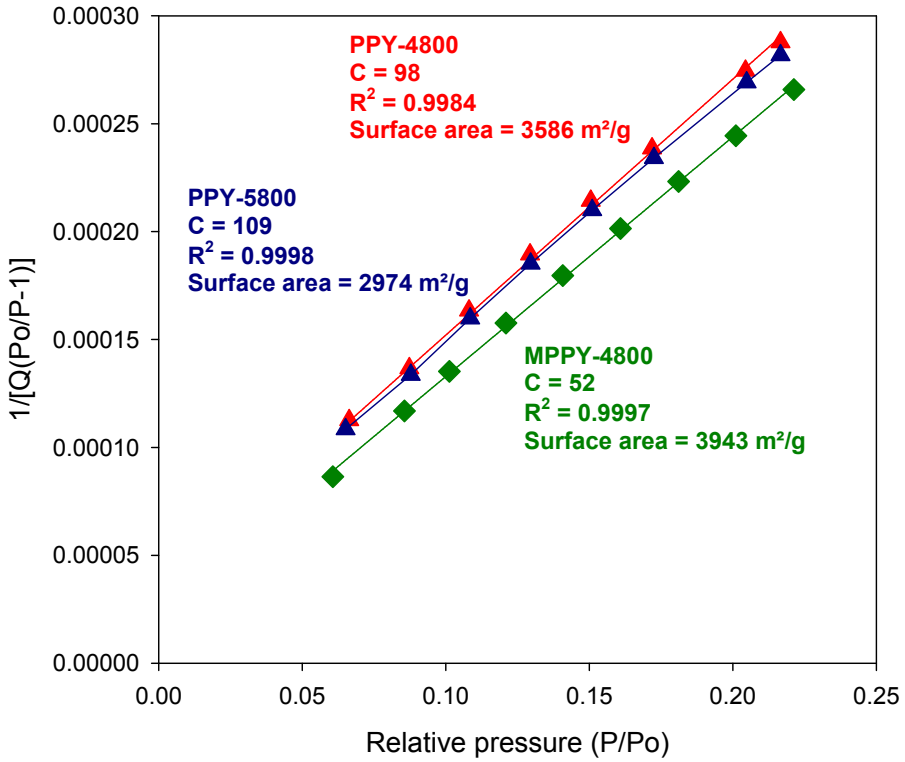

6. M. Sevilla, W. Sangchoom, N. Balahmar, A. B. Fuertes and R. Mokaya, *ACS Sust. Chem. Eng*., 2016, **4**, 4710.
7. J. He, J. W. F. To, P. C. Psarras, H. Yan, T. Atkinson, R. T. Holmes, D. Nordlund, Z. Bao and J. Wilcox, *Adv. Energy Mater*. 2016, **6**, 1502491.
8. A. S. Jalilov, Y. Li, J. Tian, J. M. Tour, *Adv. Energy Mater*. 2017, **7**, 1600693.
9. H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, J. Kim and O. M. Yaghi, *Science* 2010, **329**, 424.
10. O. K. Farha, A. O. Yazaydın, I. Eryazici, C. D. Malliakas, B. G. Hauser, M. G. Kanatzidis, S. T. Nguyen, R. Q. Snurr and J. T. Hupp, *Nat. Chem*. 2010, **2**, 944.

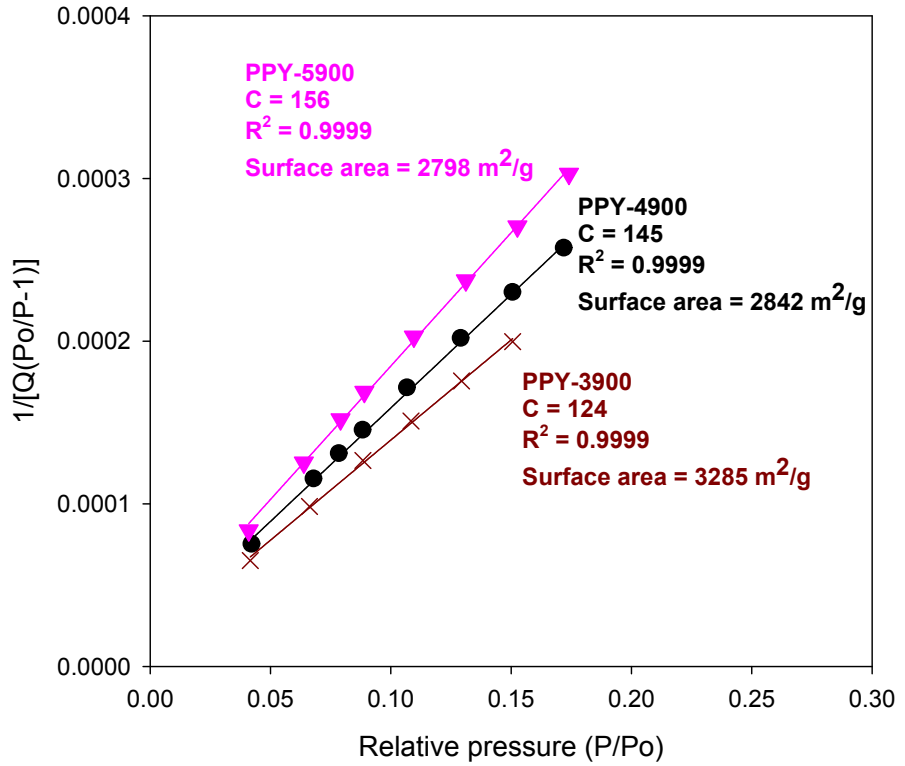



**Supporting Figure S1**. Thermogravimetric analysis (TGA) curves of polypyrrole-derived activated (PPY-xT) carbons heated in air.

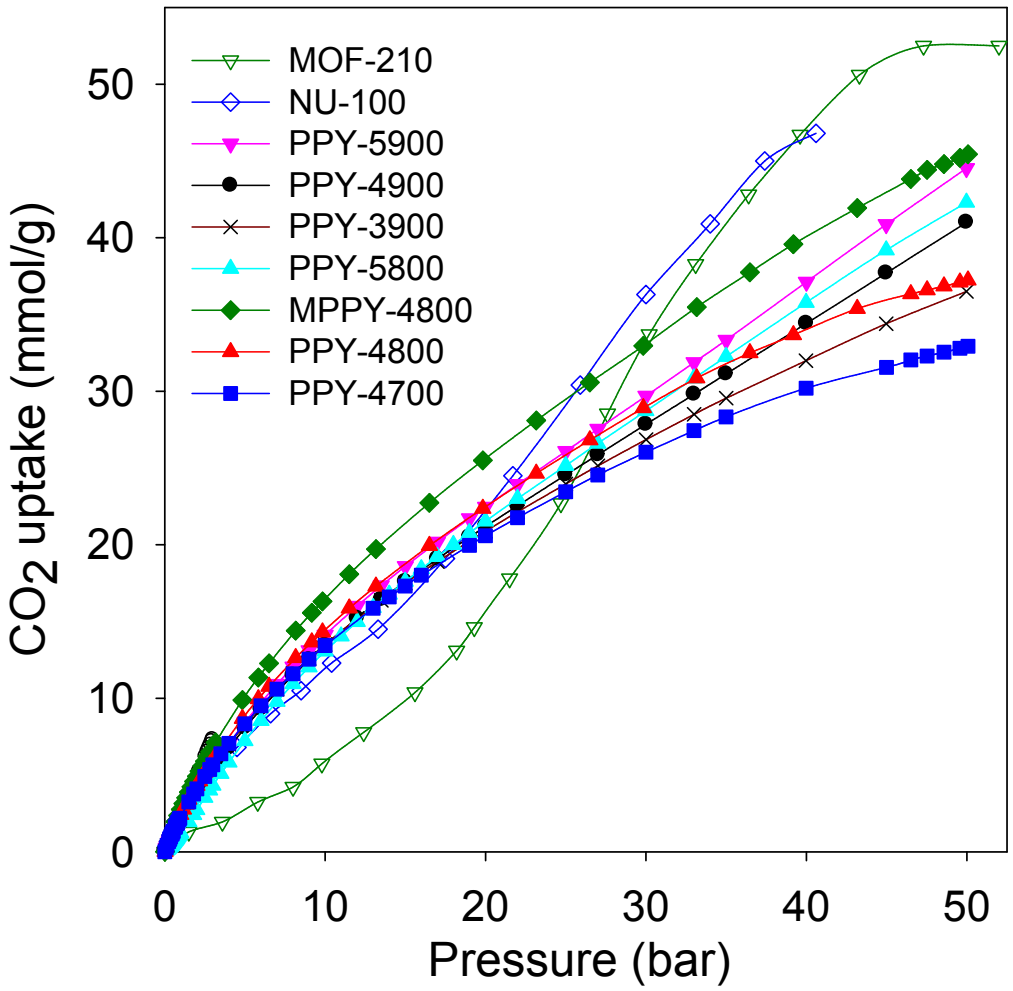



**Supporting Figure S2**. Powder XRD patterns of polypyrrole-derived activated (PPY-xT) carbons.



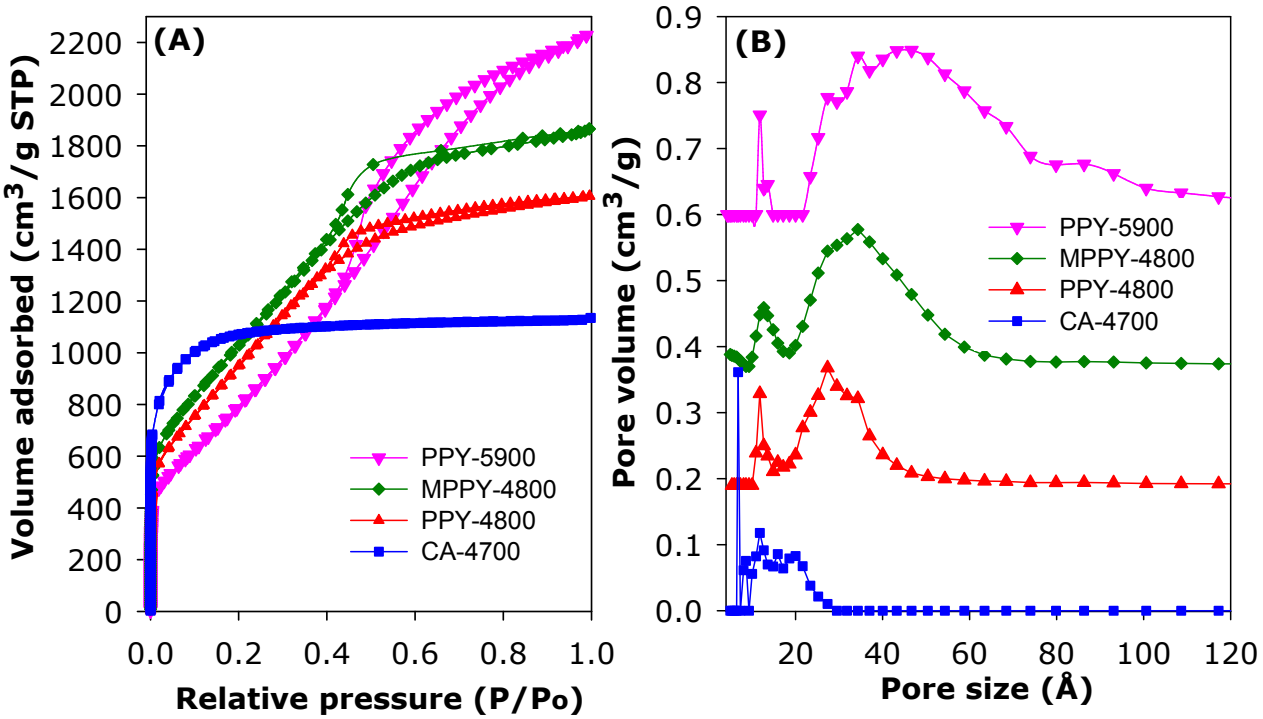

**Supporting Figure S3**. Rouquerel plots used to calculate the BET surface area of polypyrrole-derived activated (PPY-xT) carbons. We also show the values of the BET (or C) constants.



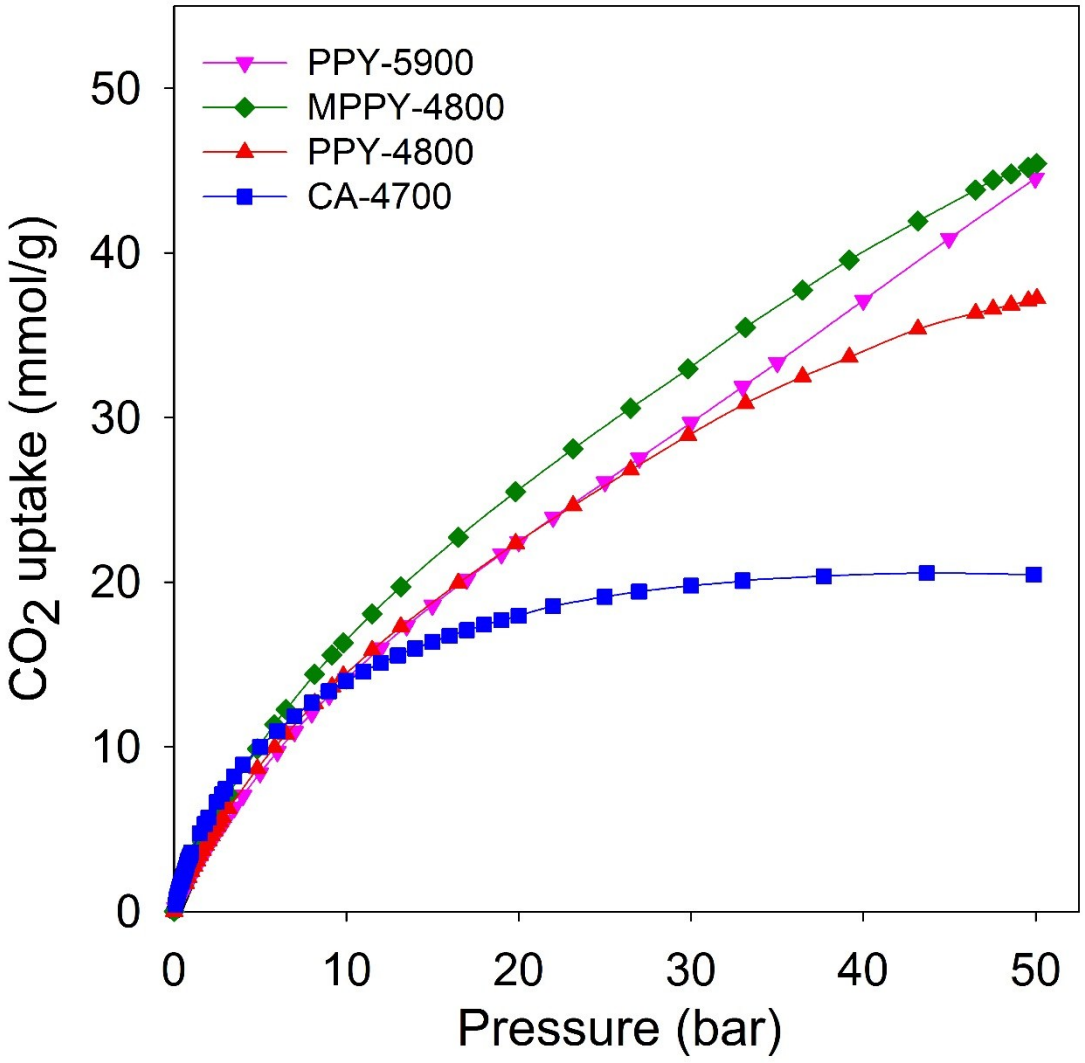

**Supporting Figure S4**. Excess $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon and benchmark MOFs (MOF-210 and NU-100)* at 25 °C and pressure of 0 – 50 bar.

*Data for MOF-210 is taken from reference 51 (O. K. Farha, A. O. Yazaydın, I. Eryazici, C. D. Malliakas, B. G. Hauser, M. G. Kanatzidis, S. T. Nguyen, R. Q. Snurr and J. T. Hupp, *Nat. Chem*. 2010, **2**, 944).

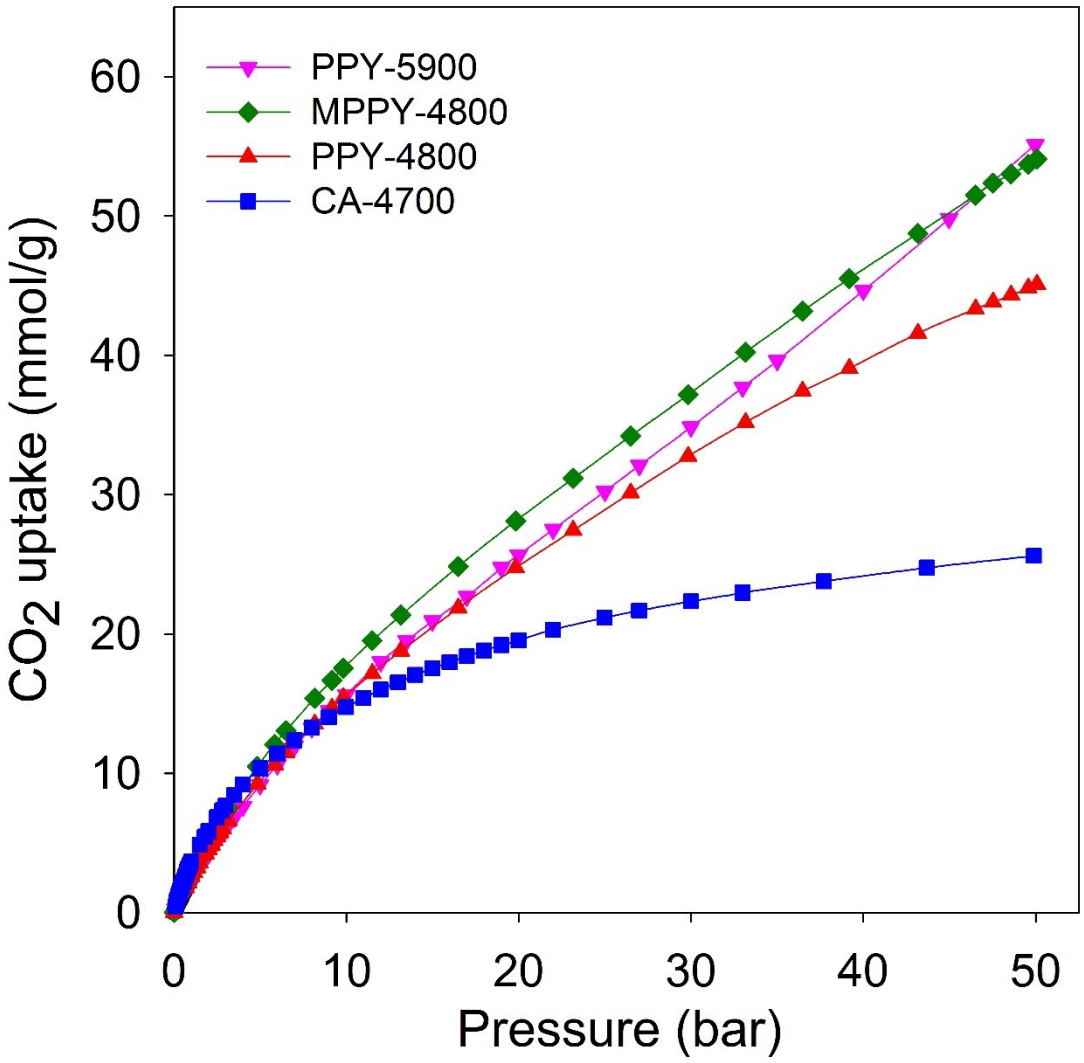
*Data for NU-100 is taken from reference 50 (H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, J. Kim and O. M. Yaghi, *Science* 2010, **329**, 424).



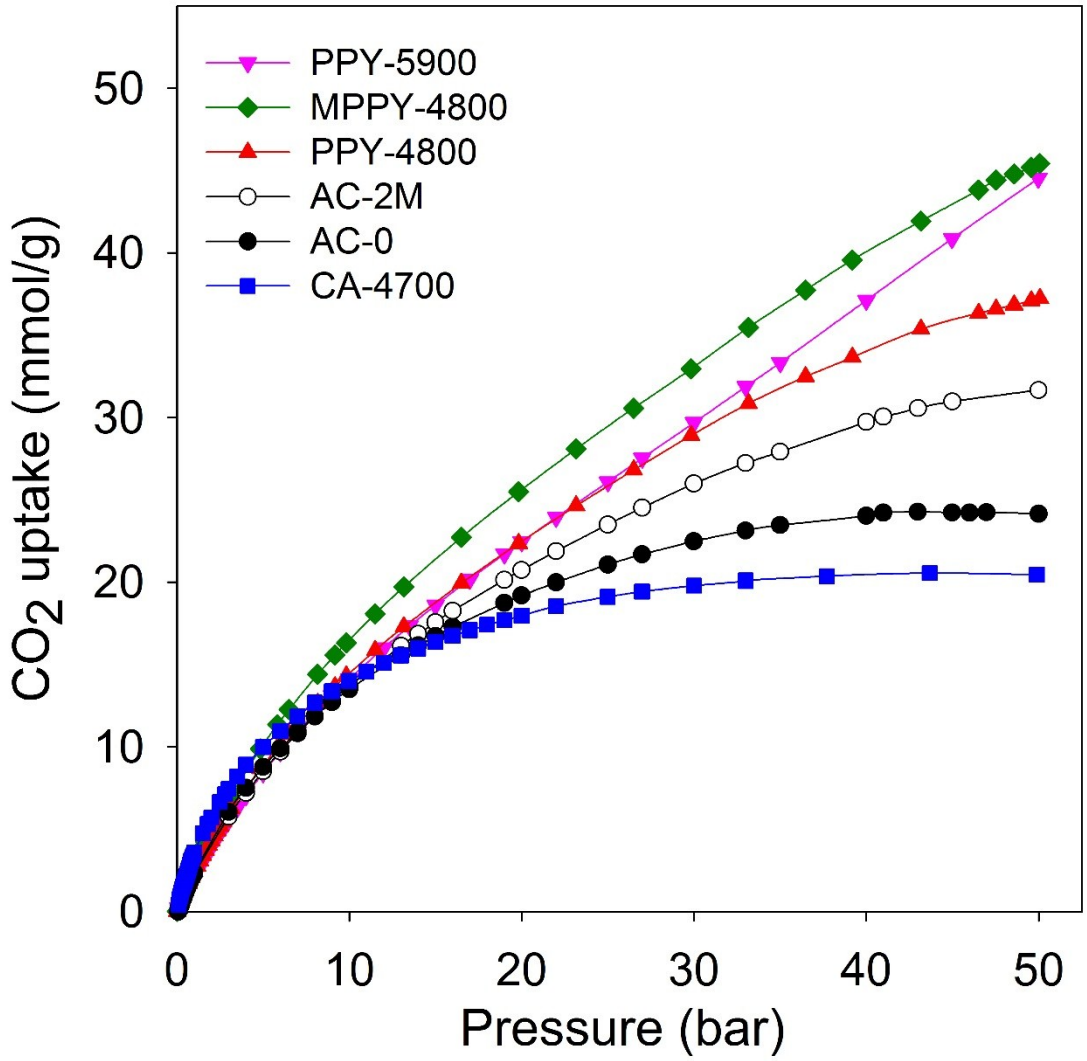

**Supporting Figure S5**. Nitrogen sorption isotherms (A) and corresponding pore size distribution (PSD) curves (B) of mesoporous polypyrrole-derived (PPY-xT) activated carbons, a compactivated (MPPY-4800) carbon, and a microporous activated carbon (CA-4700).




**Supporting Figure S6**. Excess $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon, and a microporous activated carbon (CA-4700).

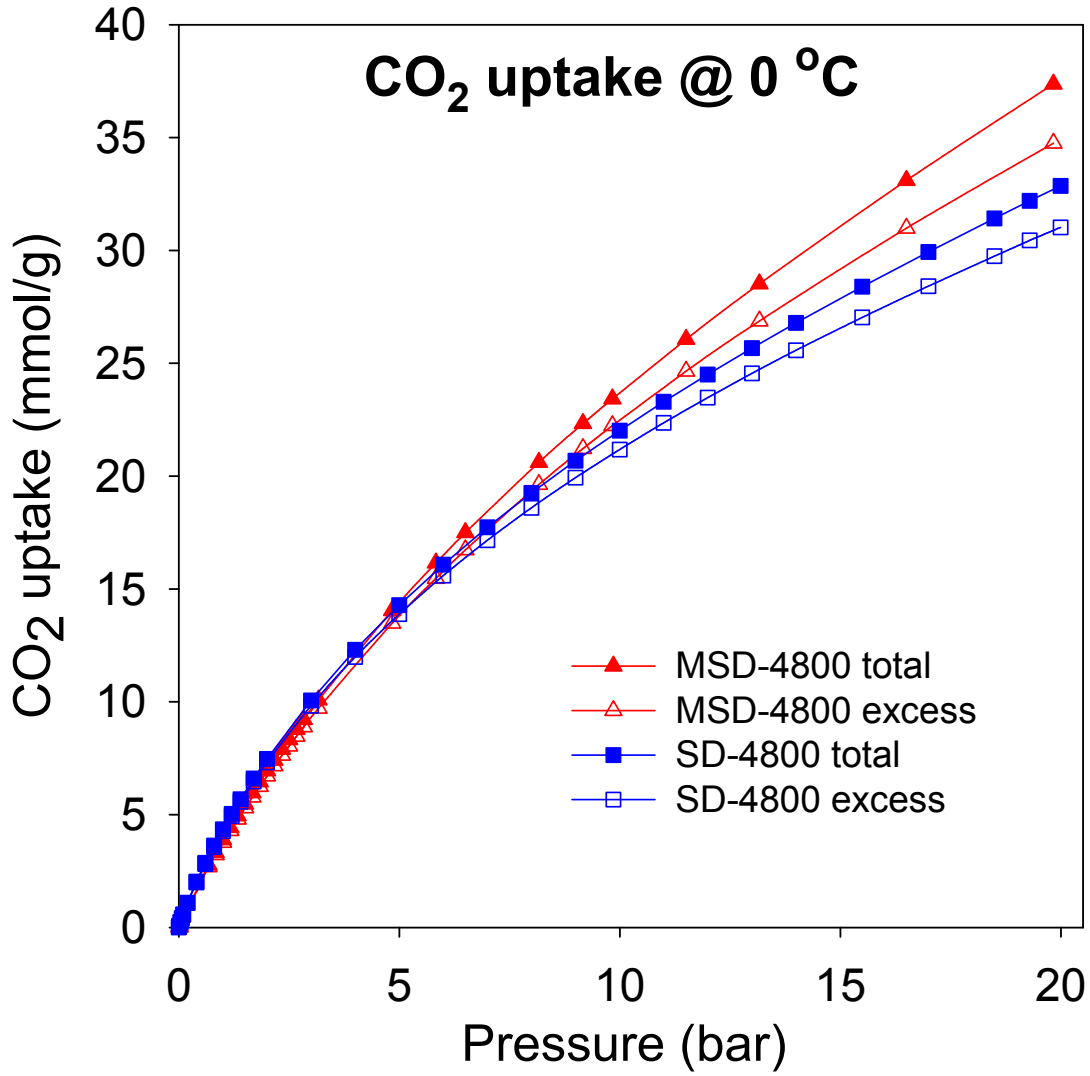



**Supporting Figure S7**. Total $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon, and a microporous activated carbon (CA-4700).

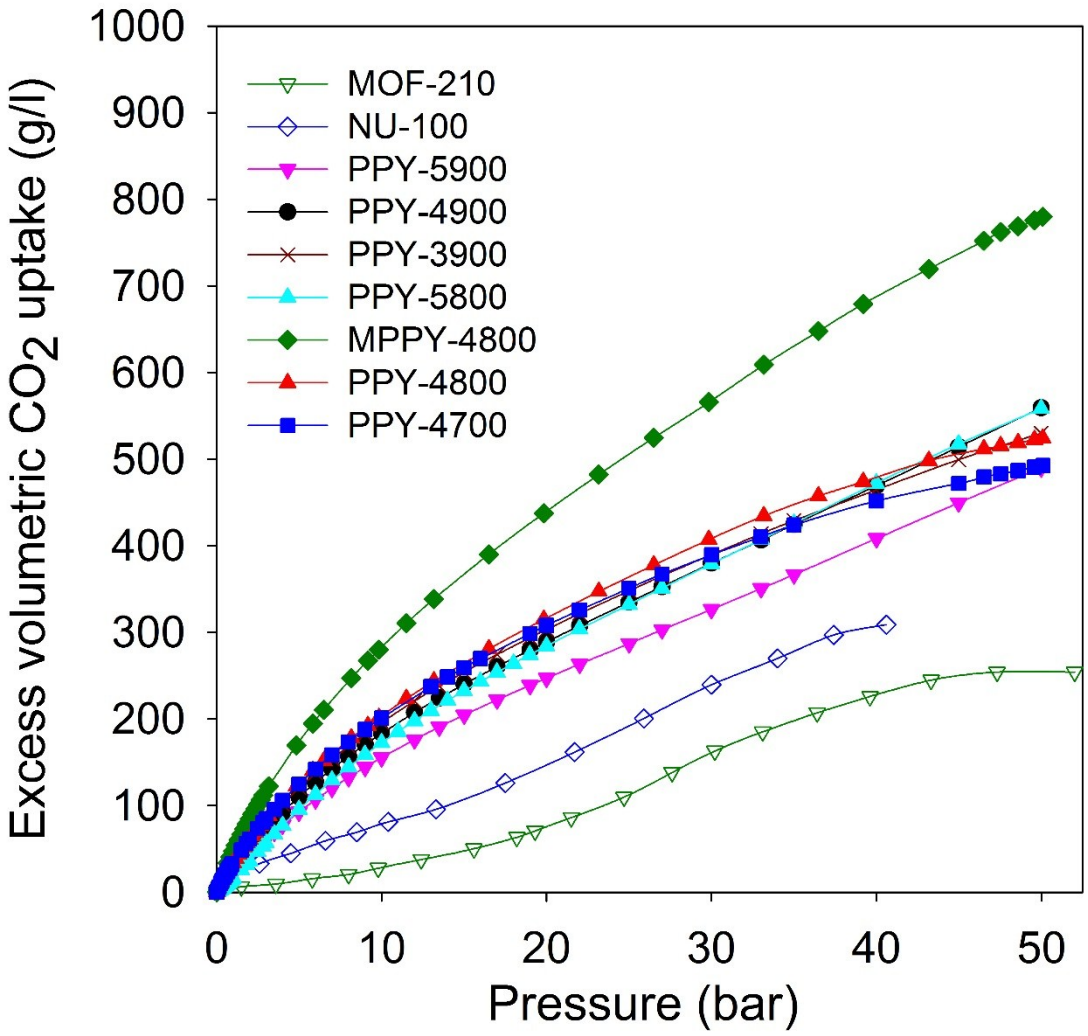



**Supporting Figure S8**. Excess $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon, a microporous activated carbon (CA-4700) and micro/mesoporous activated carbons (AC-0 and AC-2M)*.

*Data for AC-0 and AC-2M is taken from reference 37 (M. Sevilla, W. Sangchoom, N. Balahmar, A. B. Fuertes and R. Mokaya, *ACS Sust. Chem. Eng*., 2016, **4**, 4710).



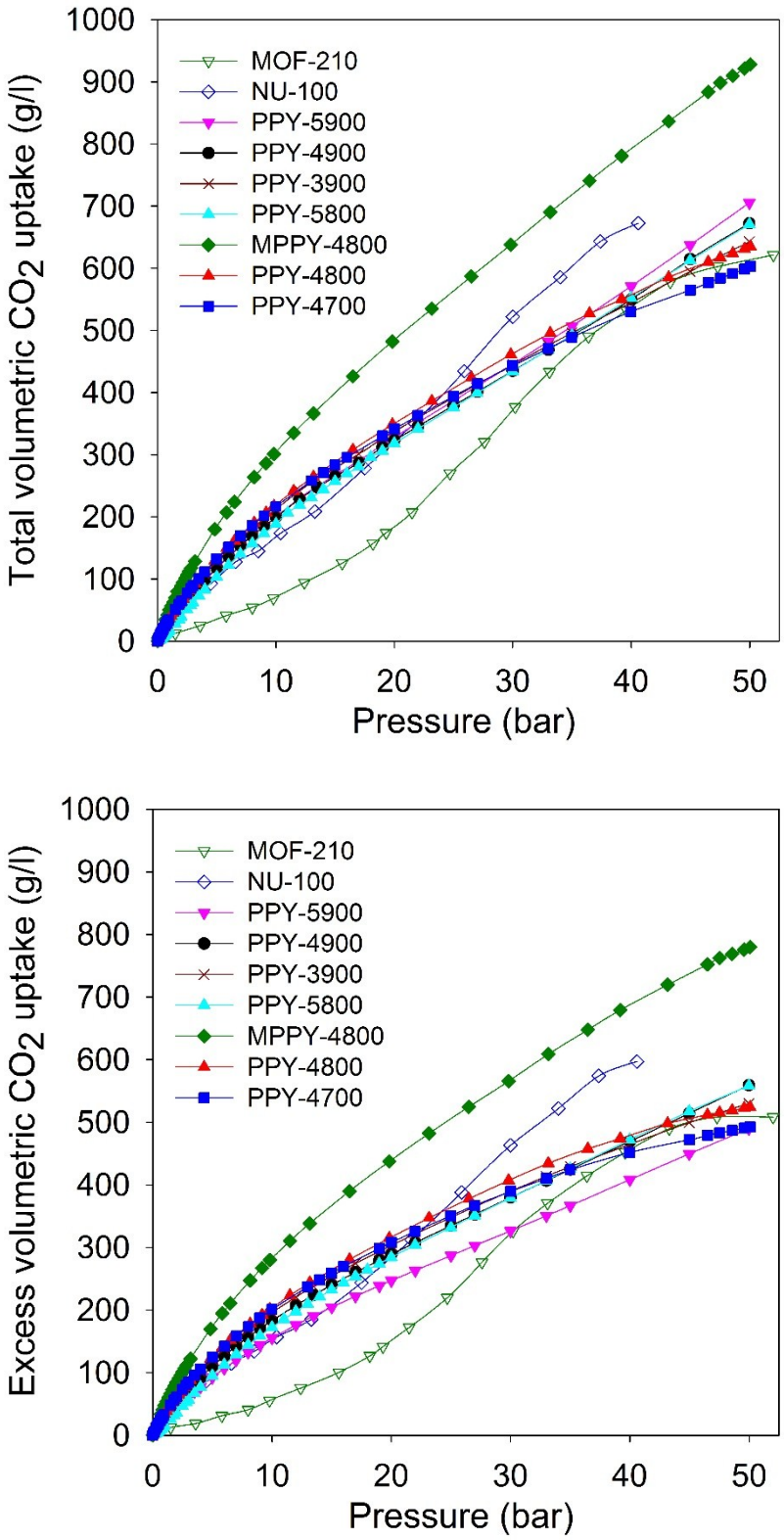

**Supporting Figure S9**. Total and excess $CO_2$ uptake at 0 °C for activated (SD-4800) and compactivated (MSD-4800) carbon derived from wood sawdust.




**Supporting Figure S10.** Excess volumetric $CO_2$ uptake of polypyrrole-derived activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon and benchmark MOFs (MOF-210 and NU-100) at 25 $^oC$ and pressure of 0 – 50 bar. Packing density values (g $cm^{-3}$) used are: 0.15 (NU-100) and 0.12 (MOF-210) according to reference 61 (Y. Peng, V. Krungleviciute, I. Eryazici, J. T. Hupp, O. K. Farha and T. Yildirim, *J. Am. Chem. Soc*. 2013, **135**, 11887–11894).

*$CO_2$ uptake ata for MOF-210 is taken from reference 51 (O. K. Farha, A. O. Yazaydın, I. Eryazici, C. D. Malliakas, B. G. Hauser, M. G. Kanatzidis, S. T. Nguyen, R. Q. Snurr and J. T. Hupp, *Nat. Chem*. 2010, **2**, 944).

*$CO_2$ uptake data for NU-100 is taken from reference 50 (H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, J. Kim and O. M. Yaghi, *Science* 2010, **329**, 424).




**Supporting Figure S11.** Total (top) and excess (bottom) $CO_2$ uptake of activated (PPY-xT) carbons, compactivated (MPPY-4800) carbon and MOFs (MOF-210 and NU-100) at 25 $^{o}$C. Crystal density of 0.25 and 0.30 g $cm^{-3}$, respectively, was used to estimate the volumetric uptake of MOF-210 and NU-100. $CO_2$ uptake data for the MOFs is adapted from reference 50 and 51.