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SUPPLEMENTARY INFORMATION

Compaction of a zirconium metal-organic framework (UiO-66) for high density hydrogen storage applications

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Content:

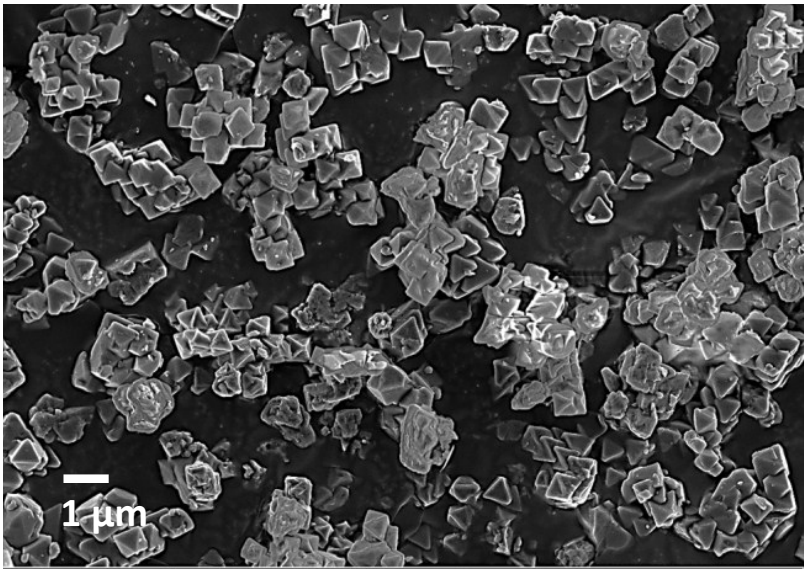

Figure S1: SEM image of UiO-66 powder before compaction.

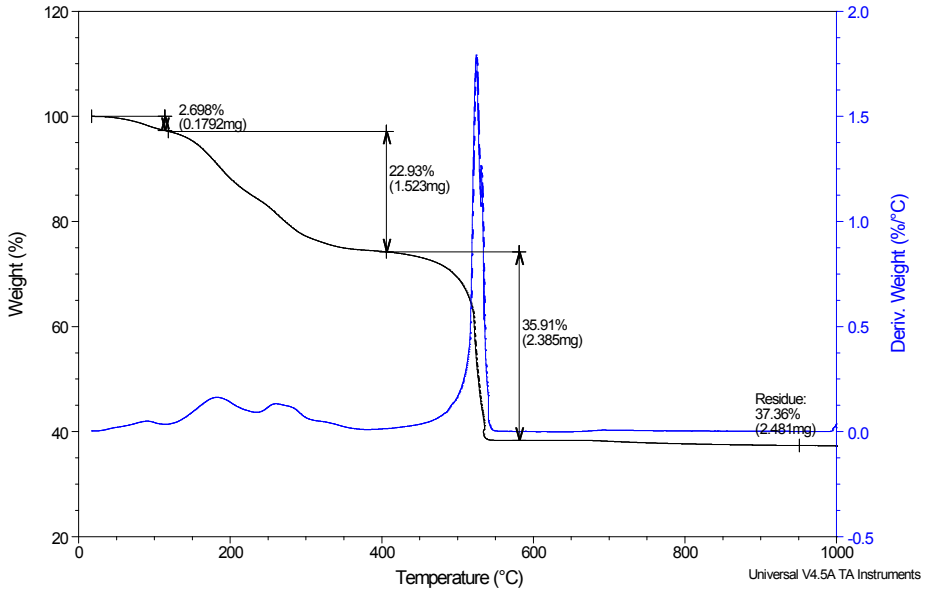

Figure S2: Thermal decomposition of UiO-66 showing multi-step decomposition from 25 up to 1000 ^{o}C under air flow.

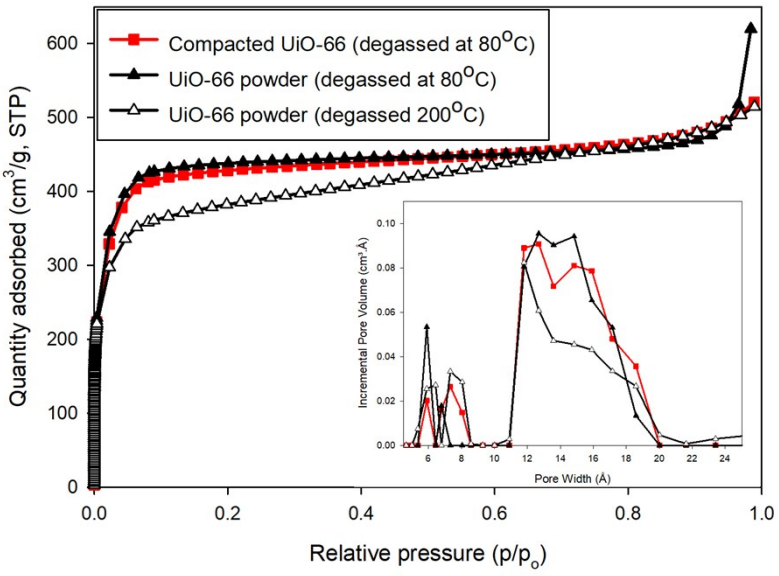

Figure S3: N_2 adsorption isotherms and pore size distribution (insert) for powdered and compacted UiO-66 crystals degassed at 80 °C and 200 °C for 32 hours under vacuum (~ 10^{-7} bar).

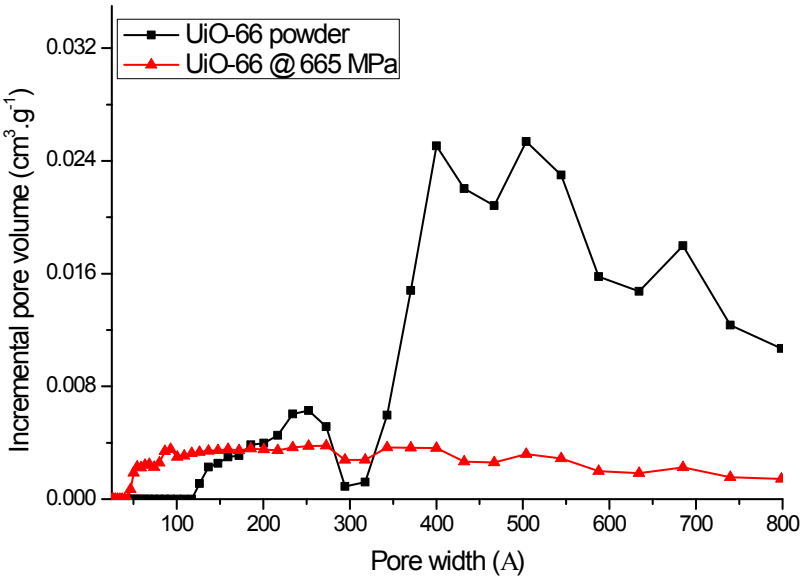

Figure S4: Pore size distribution for powdered and compacted UiO-66 in the macropore region.

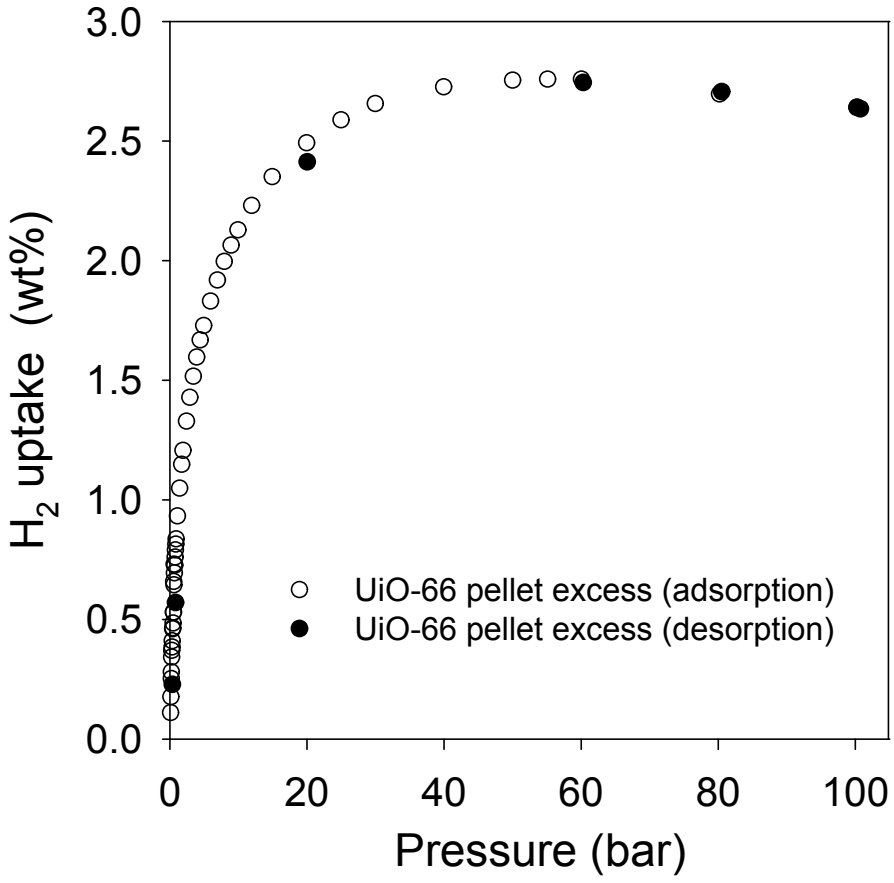

Figure S5: Excess gravimetric H_2 uptake (wt%) for compacted (i.e., pellet) UiO-66 up to 100 bar measured at 77 K showing both adsorption and desorption isotherms. The isotherms show that the uptake of H_2 is reversible.

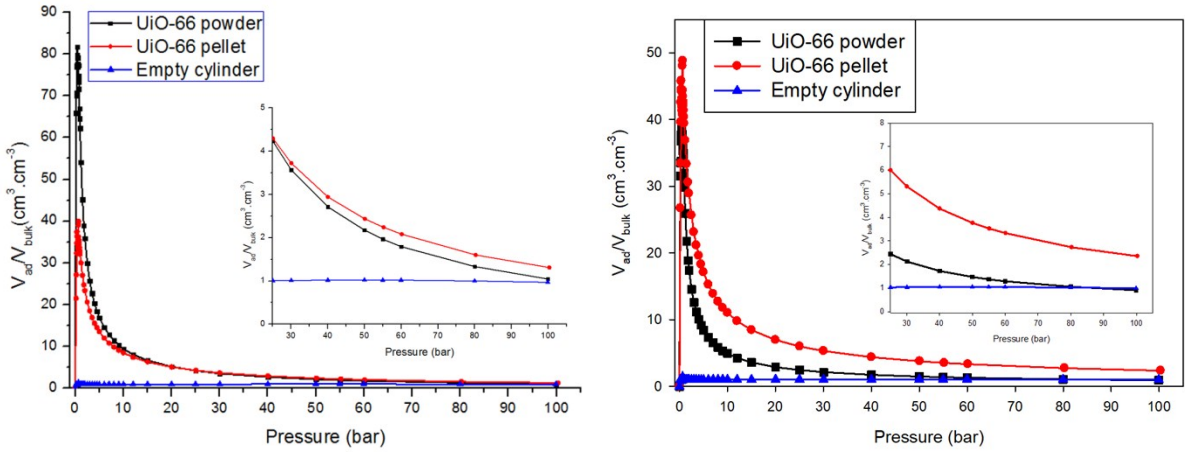

Figure S6: Adsorbed H_2 volume fractions (V_{ad}/V_{bulk}) for UiO-66 powder, UiO-66 pellet, and for an empty cylinder obtained at 77 K up to 100 bar, calculated from the ideal gas law of H_2 gas (PV = nRT).

Table S1: Comparison of textural properties for UiO-66 powder and compacted samples degassed at 80 and 200 ^{o}C for 32 hours.

Sample	BET Surface area ($m^2.g^{-1}$)	Pore volume ($cm^3.g^{-1}$)	Micropore surface area ($m^2.g^{-1}$)[a]	Micropore volume ($cm^3.g^{-1}$)[b]
UiO-66 powder (80 ^{o}C)	1737	0.96	1559 (90%)	0.60 (63%)
UiO-66 pellet (80 ^{o}C)	1707	0.81	1484 (87%)	0.57 (70%)
UiO-66 powder (200 ^{o}C)	859	0.56	671 (78%)	0.27 (48%)

[a]values in parentheses represent the percentage micropore surface area of the total BET surface area. [b]values in parentheses represent the percentage micropre volume of the total NLDFT pore volume.

Table S2: Textural properties, packing density, and H_2 uptake (at 77.3 K and 25 bar or 298 K for values in parenthesis) measured for powder and compacted UiO-66

Sample	Surface area[a] ($m^2{\cdot}g^{-1}$)	Pore volume[b] ($cm^3{\cdot}g^{-1}$)	Packing density ($g{\cdot}cm^{-3}$)	Volumetric surface area ($m^2.mL^{-1}$)[c]	Skeletal density ($g{\cdot}cm^{-3}$)	Gravimetric H_2 uptake (wt%)		Volumetric H_2 capacity ($g{\cdot}L^{-1}$)		
						Excess	Total	Excess[d]	Total[e]	Total[f]
UiO-66 Powder	1737 (1559, 90%)	0.96 (0.60, 63%)	0.57	990	1.65	2.6 (0.1)	3.4 (0.3)	15 (1)	19 (2)	34 (2)
UiO-66 Pellet	1707 (1484, 87%)	0.81 (0.57, 70%)	1.45	2475	1.78	2.6 (0.1)	3.3 (0.3)	38 (2)	48 (4)	35 (2)

[a]Values in parenthesis are micropore surface area and percentage micropore surface area of the total surface area. [b]Values in parenthesis are micropore volume and percentage micropore of the total pore volume. [c]Surface area obtained by multiplying the packing density with the BET surface area. [d]Excess volumetric capacity calculated from the packing density as per equation (2). [e]Total volumetric capacity calculated from the packing density as per equation (3). [f]Total volumetric H_2 capacity calculated using the single crystal (1.24 $g{\cdot}cm^{-3}$) and skeletal densities of UiO-66 as reported by [37]