Electronic Supplementary Material (ESI) for CrystEngComm.

Robust anionic pillared-layer framework with triphenylamine-based linkers: ion exchange and counterion-dependent sorption properties

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Supplementary Information

Crystal and framework structure of JUMP-1 with topology

Table S1: Bond lengths for the cobalt(II) ions in the crystal structure of JUMP-1 (in pm). For notation see Fig. 1 in the main text

Co1–O2	2.0380(18)
Co1–O3	2.1536(19)
Co1–O6	2.056(2)
Co2–O1	1.978(2)
Co2–O3	2.020(2)
Co2–O5	1.996(2)
Co2–O7	2.001(3)

Table S2: Bond angles at the cobalt(II) ions in the crystal structure of JUMP-1 (in deg). For notation see Fig. 1 in the main text

O2–Co1–O2A	86.51(11)	O1–Co2–O5D	102.81(9)
O2–Co1–O3B	95.03(7)	O1–Co2–O7	106.59(11)
O2–Co1–O3C	87.70(7)	O5D–Co2–O7	95.81(12)
O2–Co1–O6D	96.00(10)	O1–Co2–O3C	101.07(8)
O2–Co1–O6E	172.50(8)	O5D–Co2–O3C	114.15(8)
O3B–Co1–O3C	176.25(10)	O7–Co2–O3C	133.10(11)
O3B–Co1–O6D	85.03(8)		
O3B–Co1–O6E	92.14(8)		
O6D–Co1–O6E	82.40(15)		

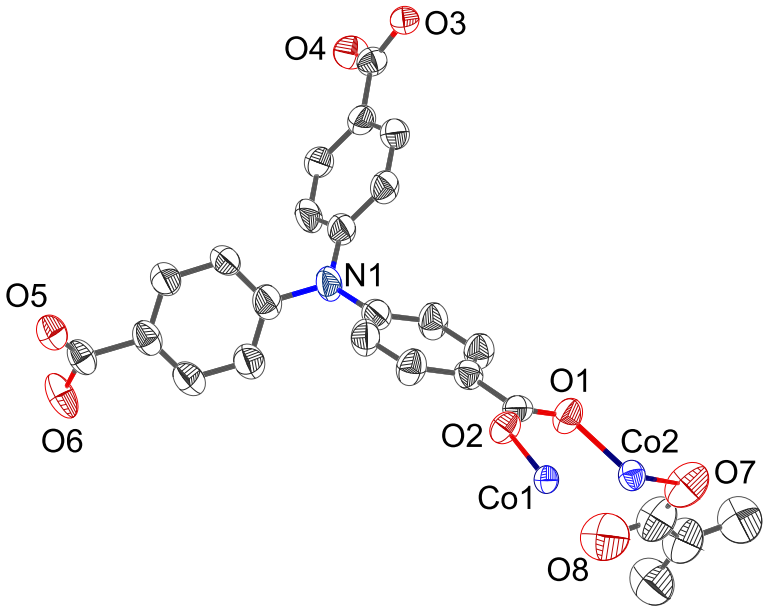

Fig. S1: Asymmetric unit of JUMP-1 with thermal ellipsoids at the 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.

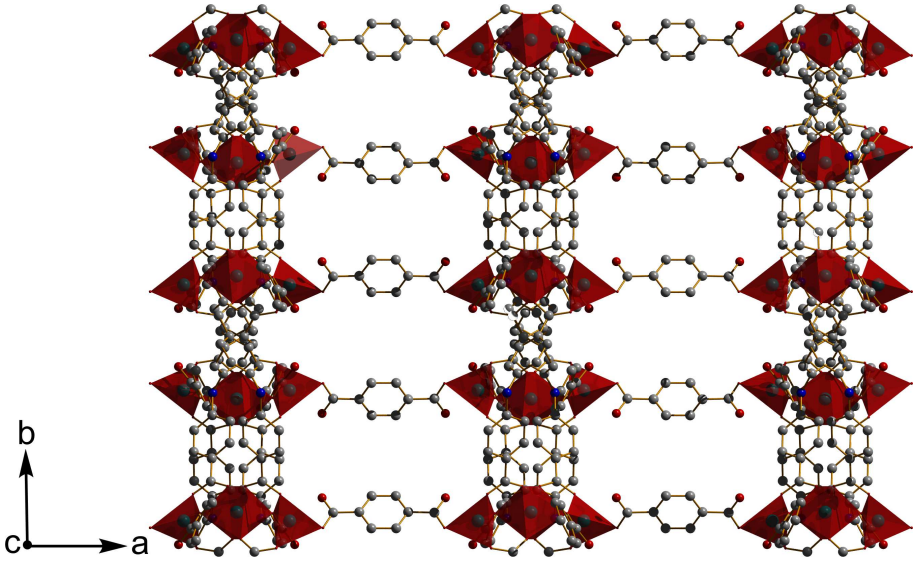

Fig. S2: 3D framework of JUMP-1 viewed along the crystallographic [001] direction. 2D networks composed of linear trinuclear cobalt(II) SBUs and ntb^{3-} ligands are arranged along the (100) plane and interconnected by the bdc^{2-} pillars. Red polyhedra represent cobalt(II) centers.

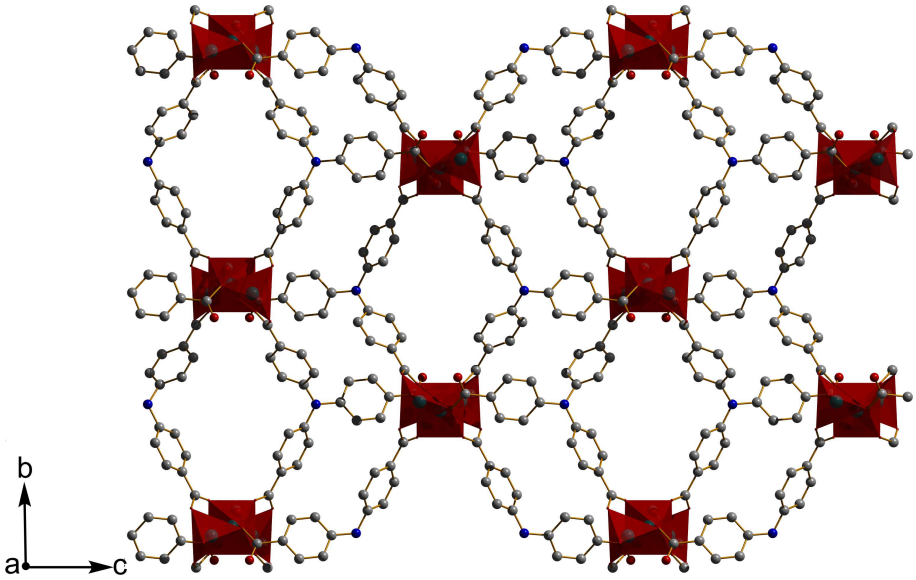

Fig. S3: Representation of the 2D network composed of linear trinuclear cobalt(II) SBUs and ntb^{3-} ligands within the 3D framework of JUMP-1 viewed along the crystallographic [100] direction.

Topological analysis for JUMP-1

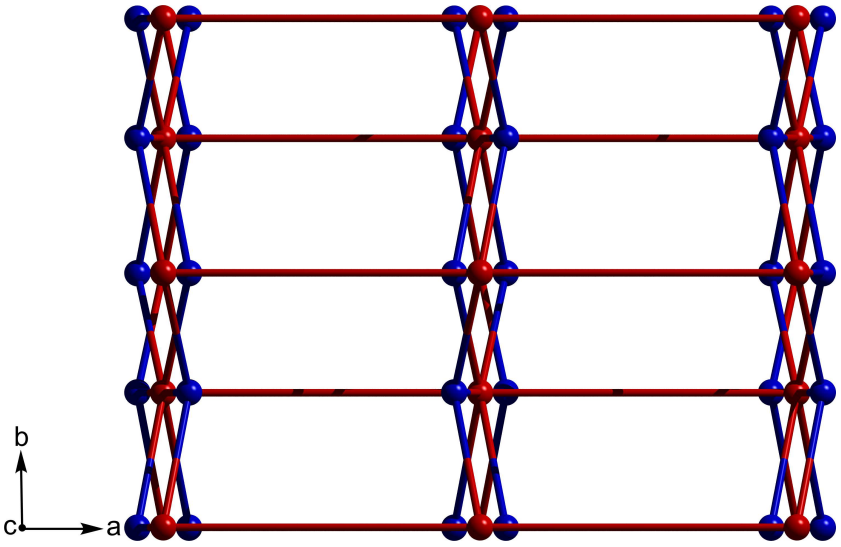

Fig. S4: Representation of the tfz-d topology of the network of JUMP-1 viewed along the negative crystallographic [001] direction. The red and blue spheres represent the trinuclear cobalt clusters (8-connected nodes) and the nitrogen atoms of the ntb^{3-} ligands (3-connected nodes), respectively.

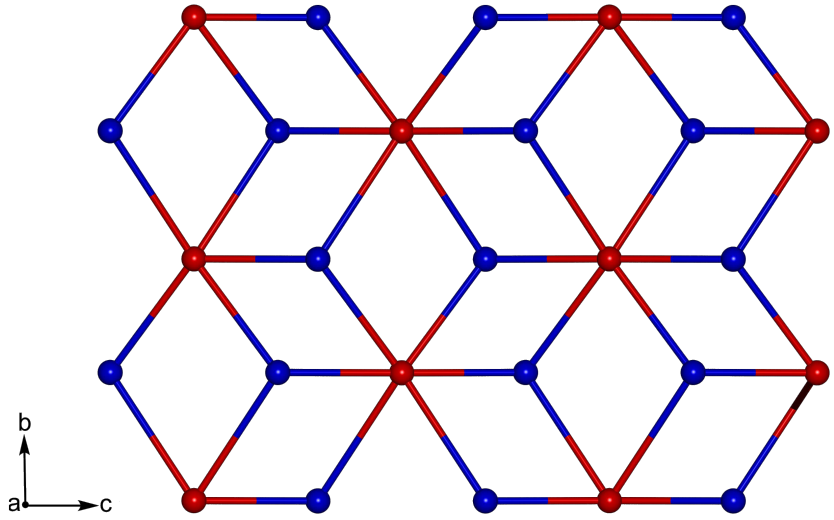

Fig. S5: Representation of the tfz-d topology of the network of JUMP-1 viewed along the crystallographic [100] direction. The red and blue spheres represent the trinuclear cobalt clusters (8-connected nodes) and the nitrogen atoms of the ntb^{3-} ligands (3-connected nodes), respectively.

Table S3: Coordination sequences for JUMP-1 (topological density $TD_{10} = 1748$)

Vertex	CS_1	CS_2	CS_3	CS_4	CS_5	CS_6	CS_7	CS_8	CS_9	CS_{10}
V1	3	18	41	74	113	164	221	290	365	452
V2	8	20	44	74	116	164	224	290	368	452

Table S4: Vertex Symbols for JUMP-1

Vertex	Vertex symbol	Extended Point Symbol
V1	$[4^3]$	[4.4.4]
V2	$[4^6.6^{18}.8^4]$	$[4.4.4.4.4.4.6_2.6_2.6_2.6_2.6_2.6_2.6_4.6_4.6_4.6_4.6_4.6_4.6_4.6_4.6_4.6_4.6_4.6_4.8_8.8_8.8_8.8_{24}]$

XRPD patterns for JUMP-1

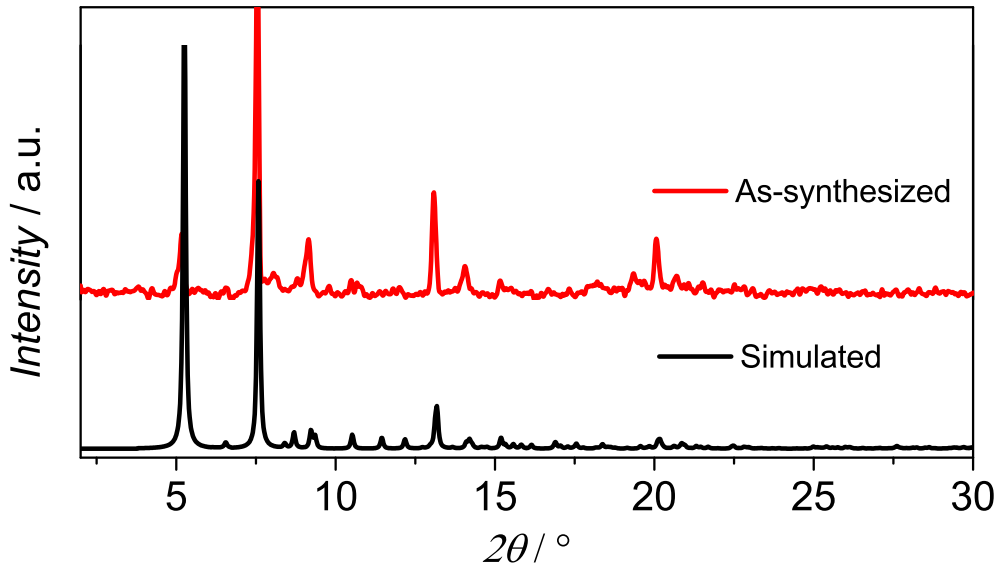

Fig. S6: XRPD pattern for JUMP-1: simulated pattern (bottom, black) and experimental pattern (top, red).

TGA profile for JUMP-1

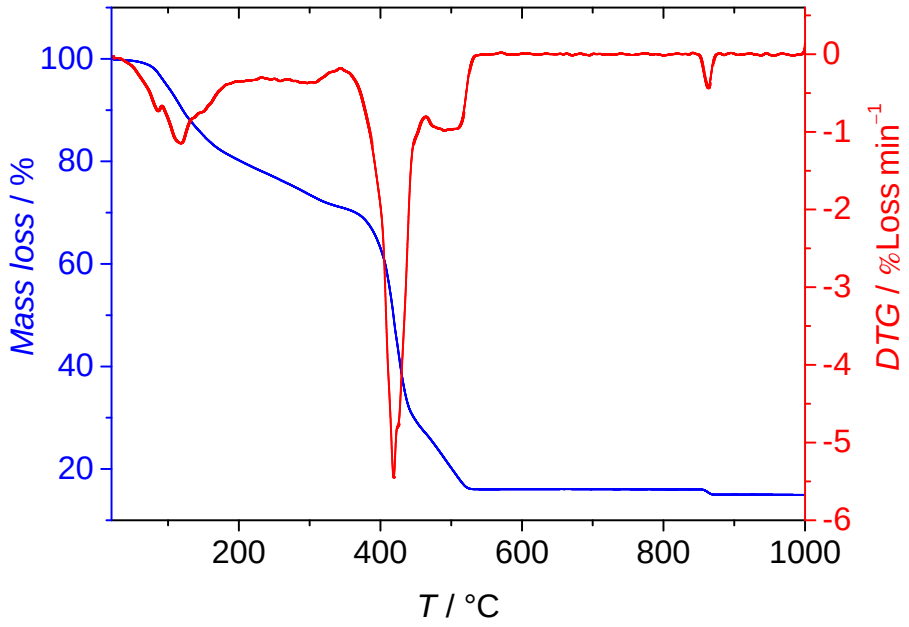

Fig. S7: Thermogravimetric data of JUMP-1: TG curve in blue and differential TG curve (DTG) in red.

Magnetic data for JUMP-1

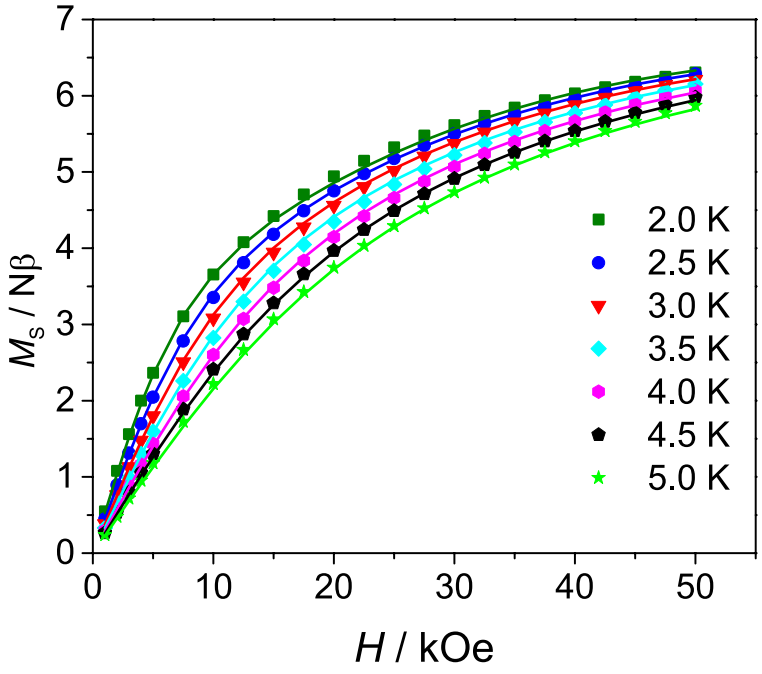

Fig. S8: Field-dependent magnetization for JUMP-1. Lines represent best fit (see text in main manuscript for parameters).

XRPD patterns for ion exchanged samples

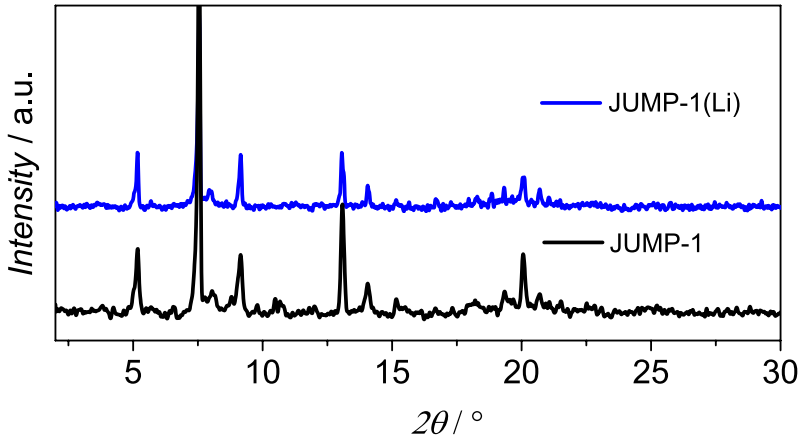

Fig. S9: XRPD pattern for lithium ion exchanged sample JUMP-1(Li) (top); for comparison also the pattern of the as-synthesized sample JUMP-1 is displayed (bottom).

TGA profile for ion exchanged sample

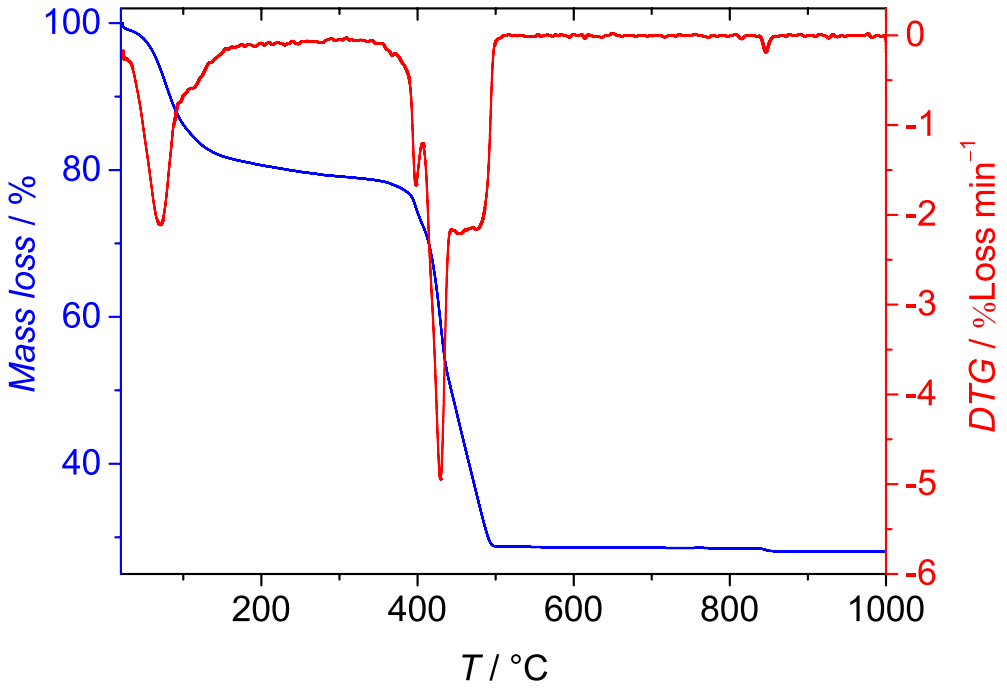

Fig. S10: Thermogravimetric data for lithium ion exchanged sample JUMP-1(Li): TG curve in blue and differential TG curve (DTG) in red.

Sorption data

Table S5: Consistency criteria derived from measured BET Data for activated samples of the as-synthesized (JUMP-1$^{\mathrm{dcm}}$ and JUMP-1$^{\mathrm{scd}}$) and lithium ion exchanged (JUMP-1(Li)$^{\mathrm{scd}}$) materials (for notation see text in main manuscript)

	$^{P}/_{P_\mathrm{o}}$ range	C	V_m [$\mathrm{cm^3/g}$]	$^{1}/_{\sqrt{C}+1}$	$^{P}/_{P_\mathrm{o}}(V_\mathrm{m})$	a(BET) [$\mathrm{m^2/g}$]	R
JUMP-1$^{\mathrm{dcm}}$	0.13 - 0.28	8.16	6.34	0.26	0.26	28	0.999
JUMP-1$^{\mathrm{scd}}$	0.08 - 0.23	134	25.96	0.08	0.08	113	0.999
JUMP-1(Li)$^{\mathrm{scd}}$	0.005 - 0.026	3025	81.52	0.018	0.018	355	0.999

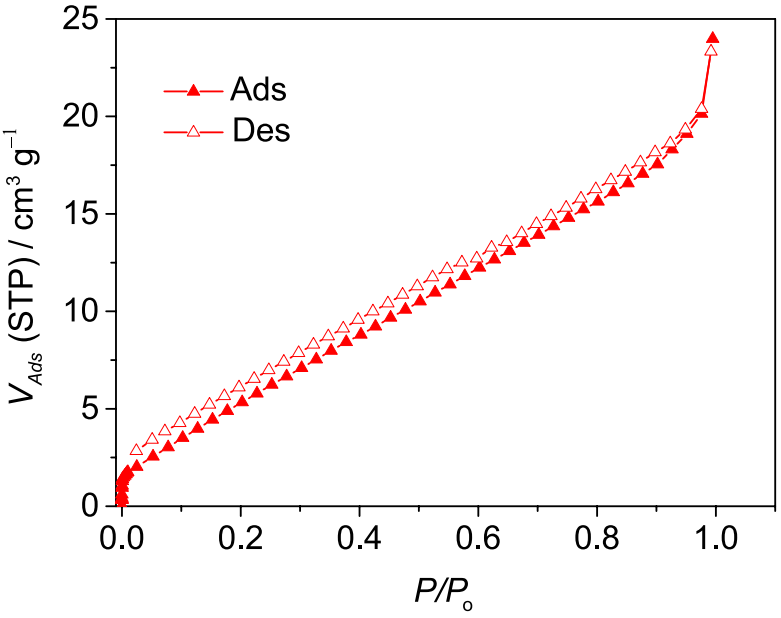

Fig. S11: N_2 isotherm for JUMP-1$^{\mathrm{dcm}}$ measured at 77 K, which is the as-synthesized sample activated by solvent-exchange with dichloromethane.

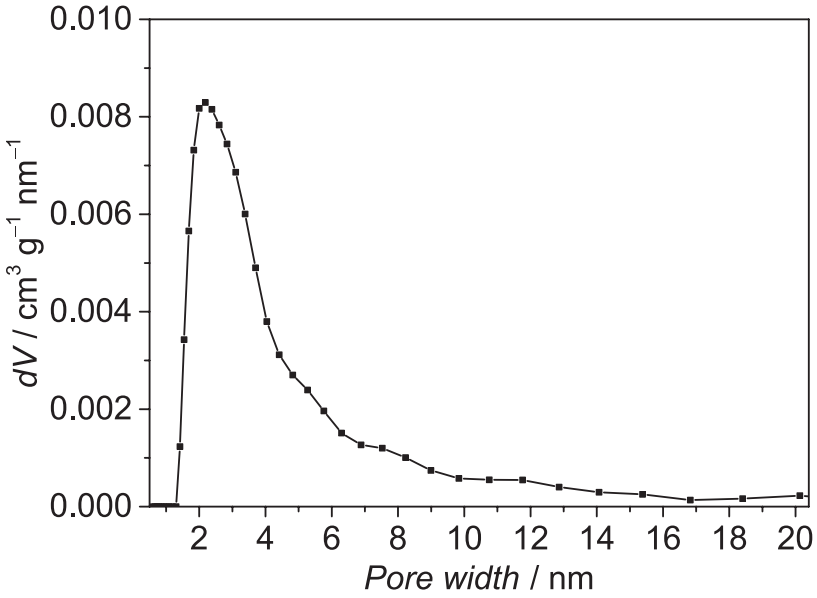

Fig. S12: Simulated pore distribution data for JUMP-1^{dcm} fitted using N_2 on carbon at 77 K (slit pores QSDFT equilibrium model).

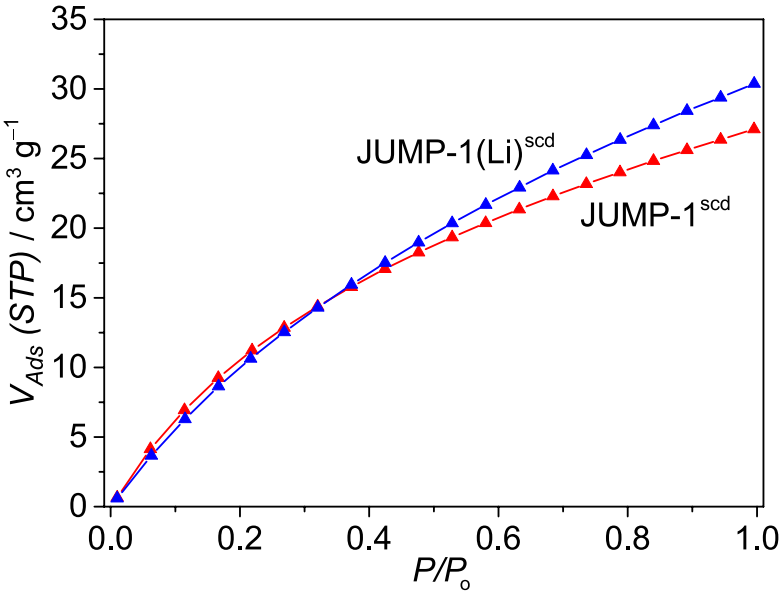

Fig. S13: CO_2 isotherms measured at 273 K for samples derived from the as-synthesized (red) and lithium ion exchanged (blue) samples of JUMP-1.