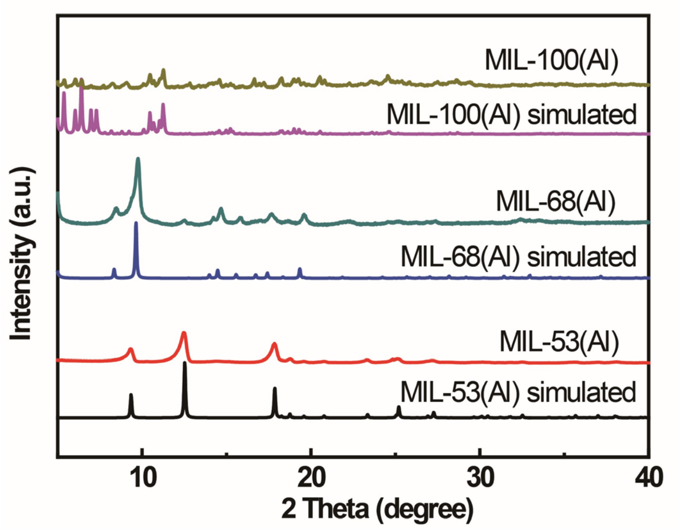
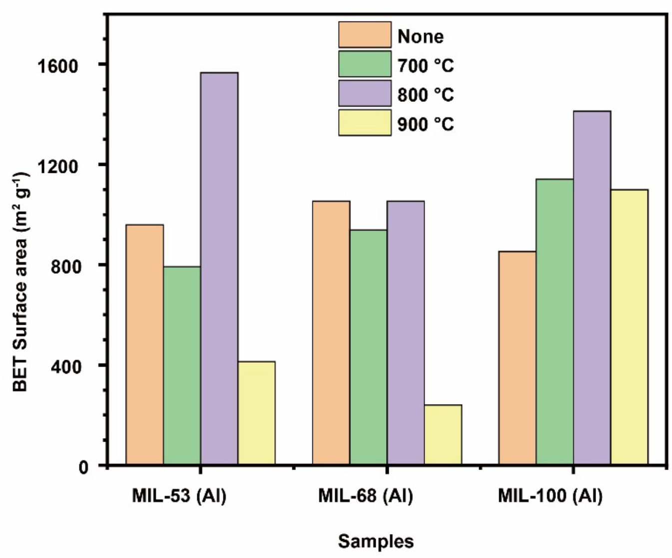
DOI: 10.20517/cs.2023.16

Pore structure unveiling effect to boost lithium-selenium batteries: selenium confined in hierarchically porous carbon derived from aluminum based MOFs.

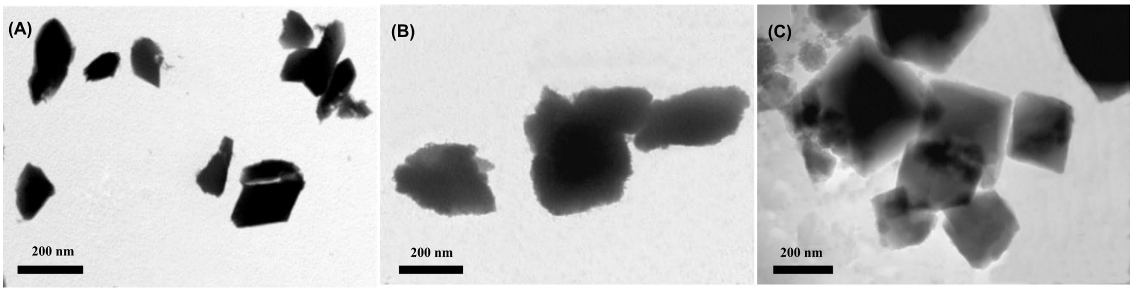


Supplementary Figure 1. XRD patterns of MIL-53 (Al), MIL-68 (Al), MIL-100 (Al) and their related simulated peaks.

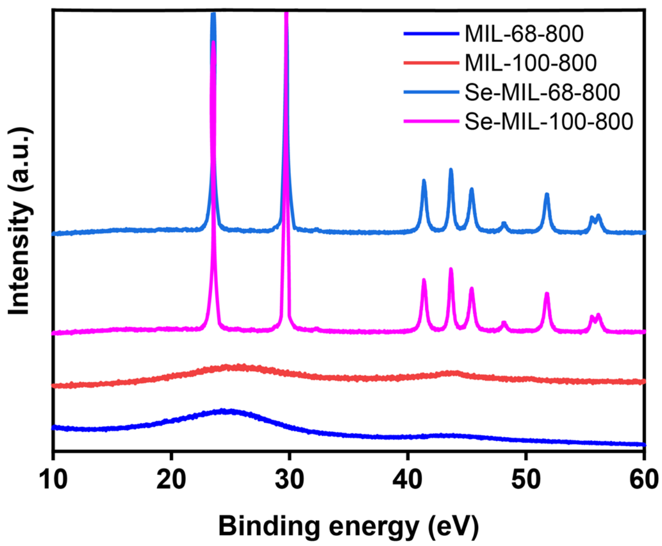
Note: Because of the very sensitive hydrothermal synthesis conditions to acidity, time, and temperature, the very small amount of MIL-96 (2θ=9.1 º and ~17º) inevitably appears in the synthesis of MIL-100[1-3].



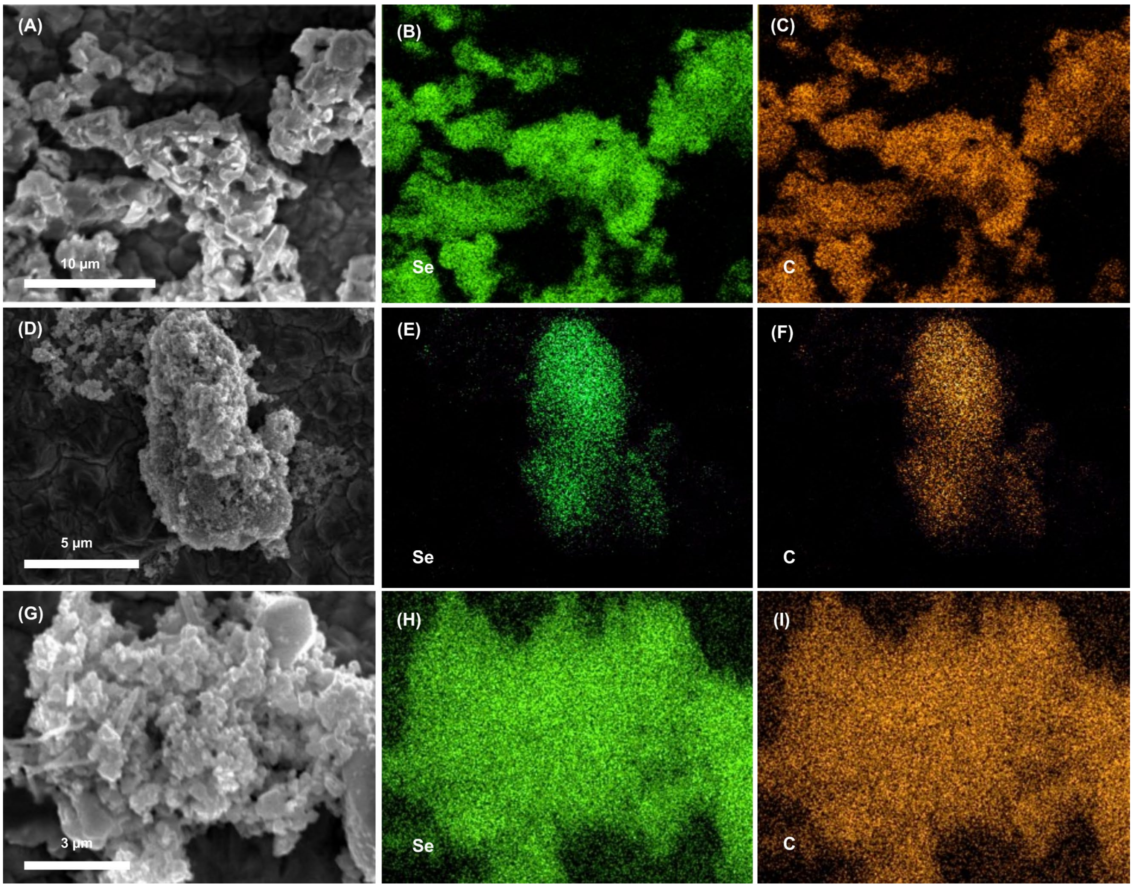
Supplementary Figure 2. Summary of the surface areas of MIL-53 MIL-68, MIL-100 at different calcination temperatures.



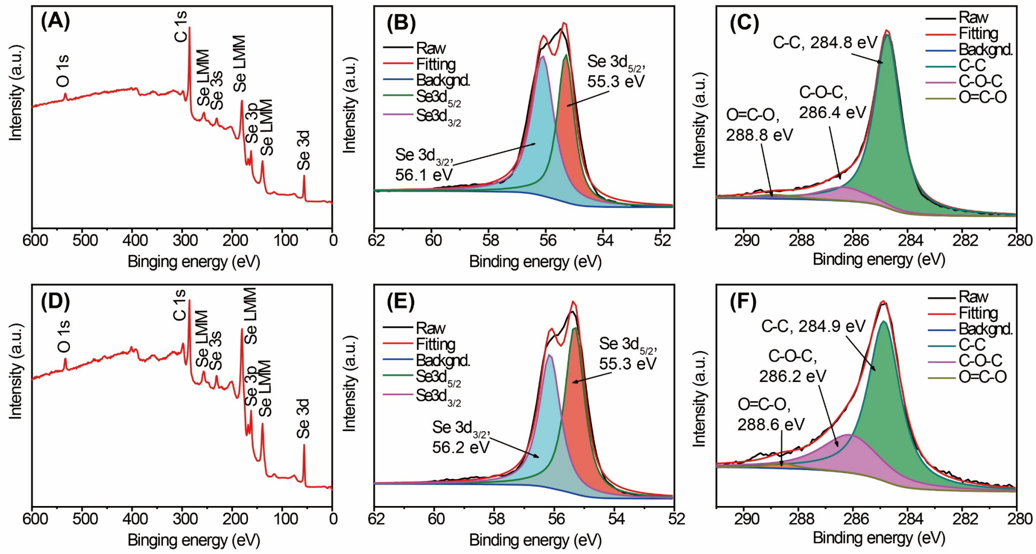
Supplementary Figure 3. TEM images of (A) MIL-53 (Al), (B) MIL-68 (Al) and (C) MIL-100 (Al).



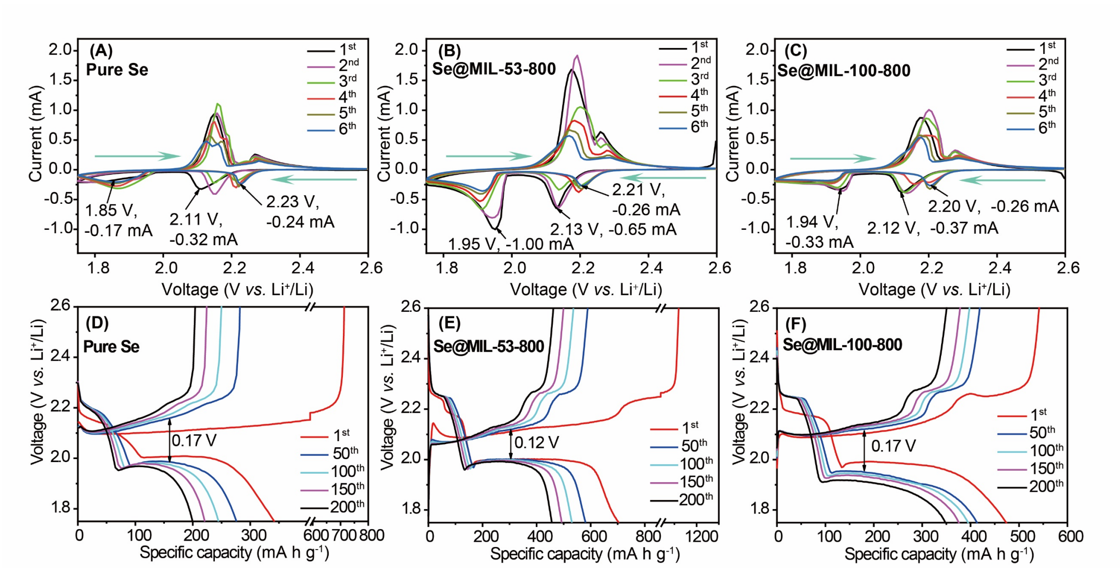
Supplementary Figure 4. XRD patterns of MIL-68-800, Se-MIL-68-800 mixture, MIL-100-800, Se-MIL-100-800 mixture.



Supplementary Figure 5. SEM images and related EDX elemental maps of Se@MIL-53-800 (A) morphology; (B) Se (green); (C) C (yellow); SEM images and related EDX elemental maps of Se@MIL-68-800 (D) morphology; (E) Se (green); (F) C (yellow); SEM images and related EDX elemental maps of Se@MIL-100-800 (G) morphology; (H) Se (green); (I) C (yellow).



Supplementary Figure 6. XPS spectrum of Se@MIL-68-800, (A) survey scan curve; high resolution (B) selenium 3d and (C) carbon 1s; XPS spectrum of Se@MIL-100-800; (D) survey scan curve; high resolution (E) selenium 3d and (F) carbon 1s.



Supplementary Figure 7. Cyclic voltammetry curves of Li-Se using (A) pure Se; (B) Li-Se@MIL-53-800; (C) Li-Se@MIL-100-800 at voltage of 1.75-2.6 V *vs*. Li^+/Li with the scan rate of 0.1 mV s^{-1}; Charge and discharge curves at different cycles of Li-Se using (D) pure Se; (E) Li-Se@MIL-53-800; (F) Li-Se@MIL-100-800 at the voltage of 1.75-2.6 V *vs*. Li^+/Li with the current density of 0.2 C.

Supplementary Table 1. The detailed BET surface area and pore volume of MIL-53(Al), MIL-68 (Al), and MIL-100 (Al) without pyrolysis and high temperature pyrolysis at 700, 800, and 900 °C, respectively.

	MIL-53 (Al)				MIL-68 (Al)				MIL-100 (Al)			
Pyrolysis temperature (°C)	None	700	800	900	None	700	800	900	None	700	800	900
BET surface area (m^2 g^{-1})	959	792	1566	413	1053	938	1053	240	852	1141	1412	1099
Pore volume (cm^3 g^{-1})	0.48	1.08	2.33	0.68	0.76	1.86	2.16	0.26	0.57	0.73	0.84	0.69

Supplementary Table 2. The detailed BET surface area and pore volume of porous carbon and after selenium encapsulation.

	MIL-53-800	Se@MIL-53-800	MIL-68-800	Se@MIL-68-800	MIL-100-800	Se@MIL-100-800
BET surface area (m^2 g^{-1})	1566	123	1053	139	1412	21
Pore volume (cm^3 g^{-1})	2.33	0.33	2.16	0.60	0.84	0.10

Supplementary Table 3. Performance comparison of Se@MIL-68-800 cathode with other Se/carbon cathode materilals of Li-Se batteries.

Cathode materials	Se loading (wt.%)	Cycling stability (mA h g^{-1})	High rate capability (mA h g^{-1})	Ref.
Se@MIL-68-800	53.5	530.1, 200 cycles, 0.2 C	300, 5 C	This work
Se@MICP	56	249, 3000 cycles, 0.1 C	241, 5 C	[14]

MHPCS/Se	48.68	260.8, 500 cycles, 0.5 C	175.4, 5 C	[20]
Meso-C@Se	48	306, 100 cycles, 0.5 C	323.8, 5 C	[36]
ARC–SiOC–Se	51.2	485, 200 cycles, 0.1 C	275.2, 2 C	[67]
Se/CPC	59.83	213.2, 100 cycles, 0.2 C	186.8, 2 C	[74]
Se/PSPC	47.7	422.3, 100 cycles, 0.2 C	221.2, 10 C	[75]
APPC/Se@PDA	61	536, 220 cycles, 0.2 C	420, 10 C	[76]

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