Supporting information

Sized-controlled ZIF-8 nanoparticle synthesis from recycled mother liquors: environmental impact assessment

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Number of pages: 8

Number of figures: 6

Number of tables: 10

Table of contents

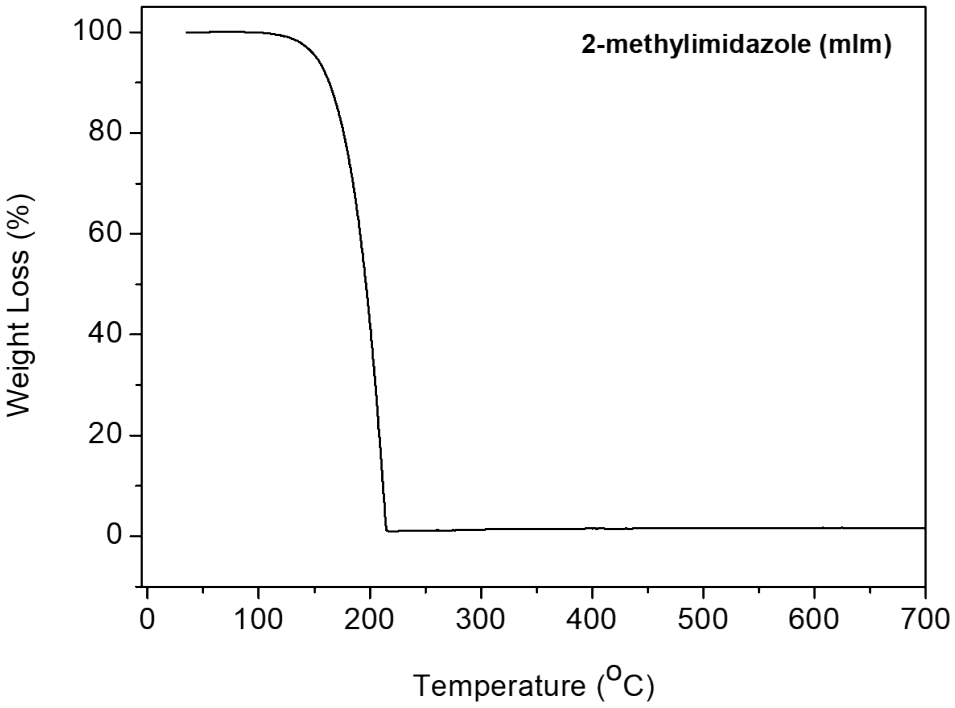

Figure S1. Thermogravimetry results of 2-methylimidazole (ligand)

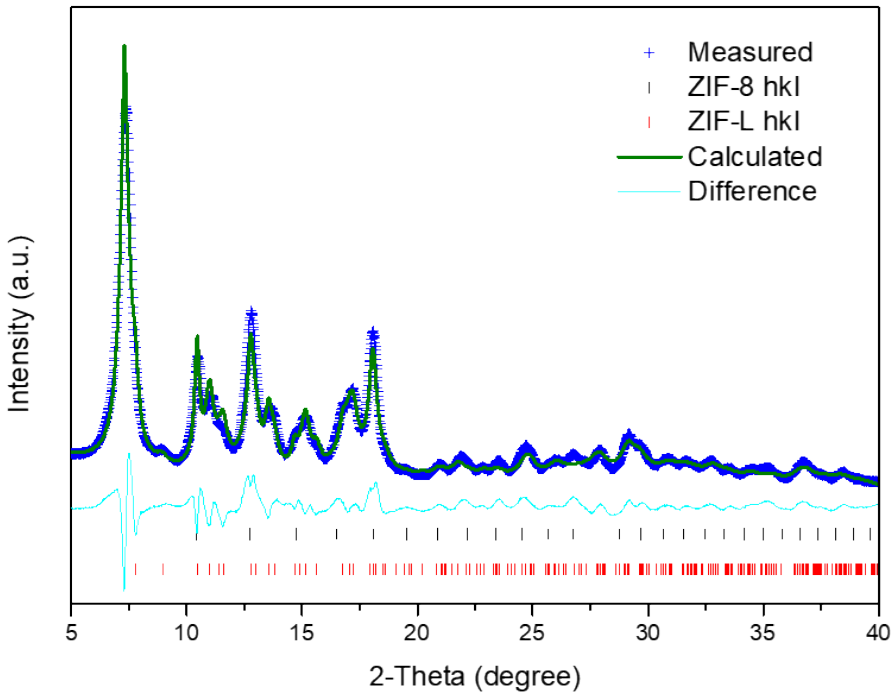

Figure S2. XRD pattern and Reitveld refinement of product A.1 done using GSAS II. Fit statistic R_{wp} = 10.42 %

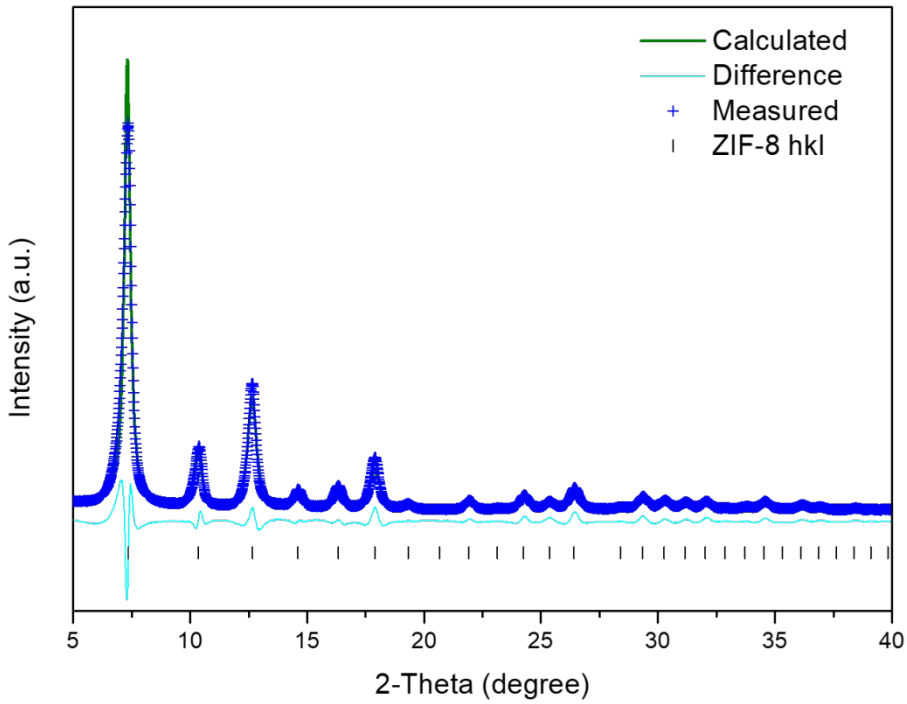

Figure S3. XRD patterns and Reitveld refinement of product A.3 done using GSAS II. Fit statistics R_{wp} = 15.47%

Table S1. Crystal lattice parameters used for the Reitveld refinements

Compound	ZIF-8	ZIF-L
Space group	I -4 3 m	C m c a
a / Å	17.0095(8)	24.11910(46)
b / Å	17.0095(8)	17.06045(33)
c / Å	17.0095(8)	19.73984(37)
Cell Volume / Å^3	4921.24	8122.6
CCDC*	864312	1509273

* Cambridge crystallographic database Code

Table S2. Atom positions calculated from Reitveld refinement for Original synthesis

Space group	I -4 3 m
a / Å	16.939
b / Å	16.939
c / Å	16.939
α / º	90
β / º	90
γ / º	90
Cell Volume / Å^3	4860.552

Table S3. Unit cell parameters calculated from Reitveld refinement for Original synthesis

Label	Element	x	y	z	frac
Zn1	Zn	0	0.5	0.75	1
N1	N	0.094	0.495	0.8062	1
C2	C	0.1215	0.512	0.8785	1
C1	C	0.132	0.6084	0.8175	1
H1	H	0.139	0.577	0.887	1
C4	C	0.0791	0.417	0.9209	1
H4A	H	0.057	0.531	0.814	0.5
H4B	H	0.122	0.78	1.114	0.5
H4C	H	0.322	0.41	0.972	0.5

Table S4. Atom positions of ZIF-8 calculated from Reitveld refinement for product A.1

Space group	I -4 3 m
a / Å	16.960
b / Å	16.960
c / Å	16.960
α / º	90
β / º	90
γ / º	90
Cell Volume / Å^3	4787.785

Table S5. Unit cell parameters of ZIF-8 calculated from Reitveld refinement for product A.1

Label	Element	x	y	z	frac
Zn1	Zn	0.5	0	0.25	1
C3	C	0.624	0.0053	0.376	1
N1	N	0.5883	-0.0357	0.3173	1
C1	C	0.6276	-0.1088	0.316	1
H1	H	0.6165	-0.1506	0.2817	1
C4	C	0.5985	0.0861	0.4015	1
H4A	H	0.557	0.1047	0.3672	0.5
H4B	H	0.6428	0.1218	0.3988	0.5
H4C	H	0.5791	0.0839	0.4551	0.5
O1	O	0.692	0.692	0.308	1
O2	O	0.816	0.816	0.184	1

Table S6. Atom positions of ZIF-L calculated from Reitveld refinement for product A.1

Space group	C m c a
a / Å	24.132
b / Å	16.899
c / Å	19.742

α / º	90
β / º	90
γ / º	90
Cell Volume / Å^3	8051.54

Table S7. Unit cell parameters of ZIF-L calculated from Reitveld refinement for product A.1

Label	Element	x	y	z	frac
Zn1	Zn	0.25	0.05545	0.25	1
Zn2	Zn	0.12592	0.3076	0.10051	1
C11	C	0.192631	0.18502	0.169324	1
C12	C	0.107139	0.174163	0.20478	1
C13	C	0.136613	0.111472	0.228753	1
C14	C	0.244739	0.219764	0.140634	1
N15	N	0.142758	0.219785	0.165943	1
N16	N	0.191557	0.122188	0.210246	1
H12	H	0.069834	0.18443	0.213023	1
H13	H	0.122365	0.069289	0.253076	1
H14A	H	0.240391	0.227311	0.092684	1
H14B	H	0.251914	0.26936	0.161963	1
H14C	H	0.275276	0.184869	0.148874	1
C21	C	0.187131	-0.070366	0.320948	1
C22	C	0.208216	-0.063042	0.428416	1
C23	C	0.236697	-0.005556	0.394787	1
C24	C	0.160398	-0.094943	0.255611	1
N25	N	0.175851	-0.102989	0.381308	1
N26	N	0.220124	-0.007642	0.327285	1
H22	H	0.210148	-0.073566	0.474629	1
H23	H	0.262463	0.028698	0.413651	1
H24A	H	0.168355	-0.149252	0.247121	1
H24B	H	0.120972	-0.087673	0.25876	1
H24C	H	0.174759	-0.063634	0.219147	1
C31	C	0	0.293683	0.095884	1
C32	C	0.0285	0.410237	0.126364	1
C34	C	0	0.212076	0.068055	1
N35	N	0.0461	0.334403	0.111144	1
H32	H	0.05126	0.453166	0.134976	1
H34A	H	0.01951	0.211263	0.025621	0.5
H34B	H	0.01804	0.177512	0.099552	0.5
H34C	H	-0.03755	0.195058	0.061128	0.5
C41	C	0.109484	0.301873	-0.053537	1
C42	C	0.141438	0.19848	-0.001083	1
C43	C	0.129253	0.177824	-0.06644	1
C44	C	0.091239	0.384281	-0.067756	1
N45	N	0.133131	0.278973	0.004597	1
N46	N	0.11474	0.246255	-0.10076	1
H42	H	0.153125	0.164888	0.033231	1
H43	H	0.12955	0.12843	-0.08417	1

H44A	H	0.106935	0.42031	-0.035629	1
H44B	H	0.102817	0.39849	-0.112688	1
H44C	H	0.051486	0.386254	-0.065013	1
H46	H	0.110099	0.251592	-0.143753	0.589
C51	C	0	0.259362	0.308363	0.823
C52	C	0.0284	0.380839	0.314675	0.823
C54	C	0	0.171427	0.308065	0.823
N55	N	0.0455	0.303716	0.303422	0.823
H52	H	0.05131	0.424139	0.320992	0.823
H55	H	0.07869	0.287921	0.294992	0.411
H54A	H	0.032898	0.151104	0.329596	0.411
H54C	H	0	0.154125	0.261757	0.411
O11	O-2	0.0322	-0.013	0.0579	0.5
O16	O-2	0.1061	0.5076	0.4466	0.353

Table S8. Atom positions of ZIF-8 calculated from Reitveld refinement for product A.3

Space group	I -4 3 m
a / Å	17.317
b / Å	17.317
c / Å	17.317
α / º	90
β / º	90
γ / º	90
Cell Volume / Å^3	5192.95

Table S9. Unit cell parameters of ZIF-8 calculated from Reitveld refinement for product A.3

Label	**Element**	**x**	**y**	**z**	**frac**
Zn1	Zn	0.5	0	0.25	1.092
C3	C	0.624626	-0.026644	0.375374	1.099
N1	N	0.583529	-0.026403	0.323334	1.027
C1	C	0.62541	-0.086968	0.321034	1.004
H1	H	0.391195	-0.177687	0.337322	0.205
C4	C	0.605883	0.073919	0.394117	0.797
H4A	H	0.891395	-0.080693	0.403958	-0.62
H4B	H	0.434178	0.080895	0.365372	-0.897
H4C	H	-0.672335	-0.608748	-0.098628	-0.31
O1	O	0.643977	0.643977	0.356023	0.392
O2	O	0.800451	0.800451	0.199549	-0.727

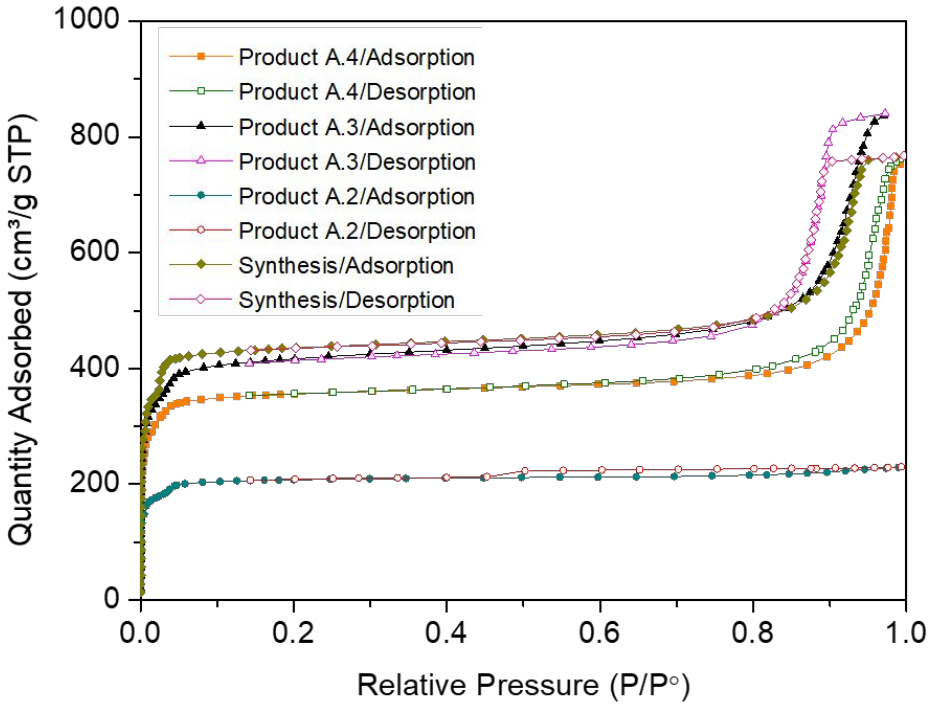

Figure S4. N_2 adsorption (full symbols) and desorption (empty symbols) isotherms for the ZIF-8 synthesis, and products A.2, A.3, and A.4

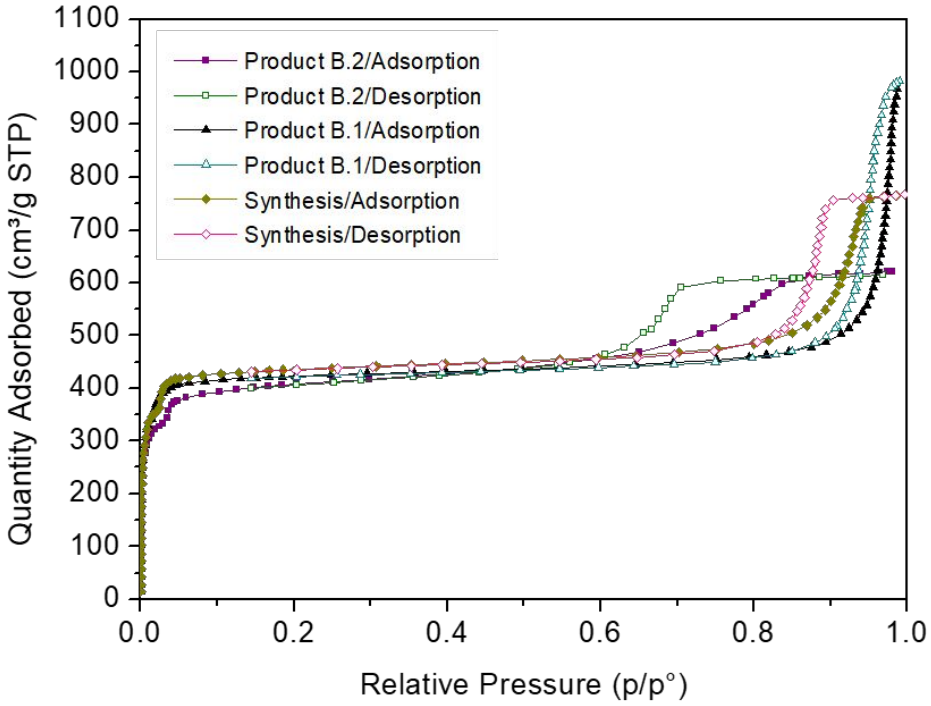

Figure S5. N_2 adsorption (full symbols) and desorption (empty symbols) isotherms for the ZIF-8 synthesis, and products B.1 and B.2

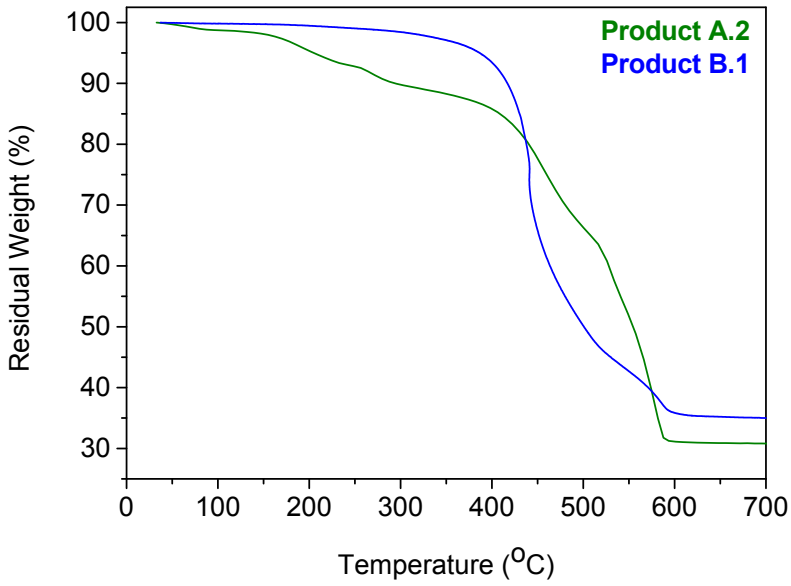

Figure S6. Thermogravimetric comparison of product A.2 and B.1

Table S10. Green metrics factors for each recycling step in product A.3

Radial pentagon	Ideal process	Experimental process (Product A.3)					
		Synthesis	Recycled 1	Recycled 2	Recycled 3	Recycled 4	Recycled 5
AE [-]	1	0.60	0.64	0.60	0.60	0.60	0.60
RME [-]	1	0.09	0.13	0.17	0.20	0.22	0.24
MRP [-]	1	0.97	0.97	0.97	0.97	0.97	0.97
1/SF [-]	1	0.38	0.40	0.44	0.45	0.46	0.47
RY [-]	1	0.40	0.53	0.67	0.75	0.82	0.88