

SUPPLEMENTARY MATERIAL

Cadmium oxide/alkali metal halide mixtures - a potential high capacity sorbent for pre-combustion CO₂ capture

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1 Nitrogen adsorption isotherm and pore size distribution

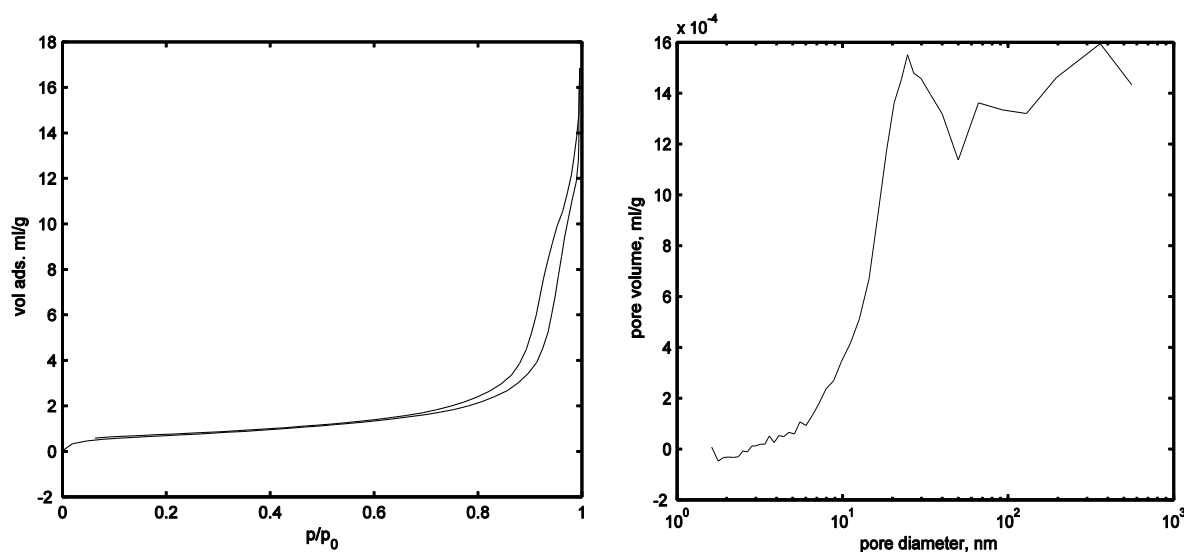


Figure A: a. N₂ adsorption-desorption isotherm (gas volume at STP adsorbed vs. p/p_0), b. BJH pore volume of a 17.5 % NaI sample, after initial calcination at 500 °C in air 3 h

2 Le Bail fit of the XRD data

2.1 Statistics

The statistical values of the Le Bail fits performed in the paper are given in Table A.

Table A: Statistics of the Le Bail fits

sample	reference in supplement	wRp	Rp	χ^2
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17.5 % NaI, calcined 500 °C air	Figure B	0.1663	0.1109	5.891
pure CdO	Figure C	0.1145	0.0740	2.930
pure CdCO ₃	Figure D	0.1245	0.0875	1.529

2.2 Le Bail fit graphs

The graphs of the Le Bail refinements of the powder XRD data are given in the figures below. The black crosses denote the observed, the red line the refined data. The background is plotted green; blue denotes the difference between calculated and observed. The difference graph is offset below the other graphs.

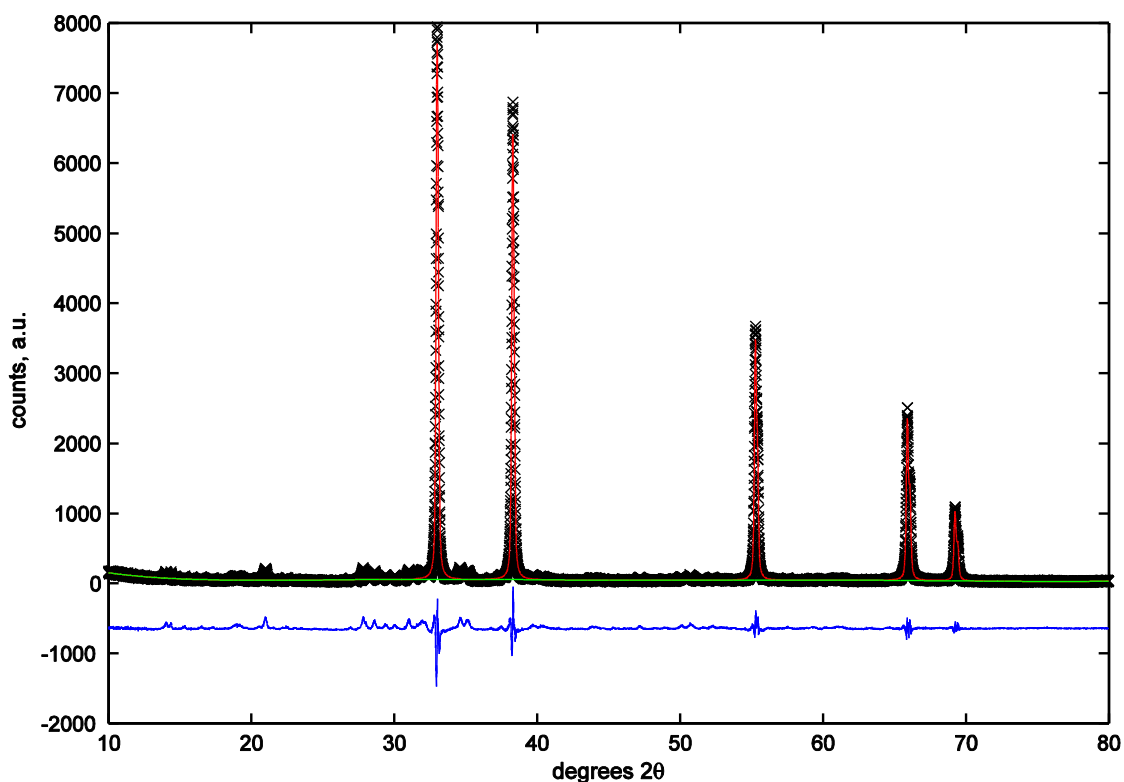


Figure B: Le Bail refinement plot of 17.5 % NaI sample, as synthesised

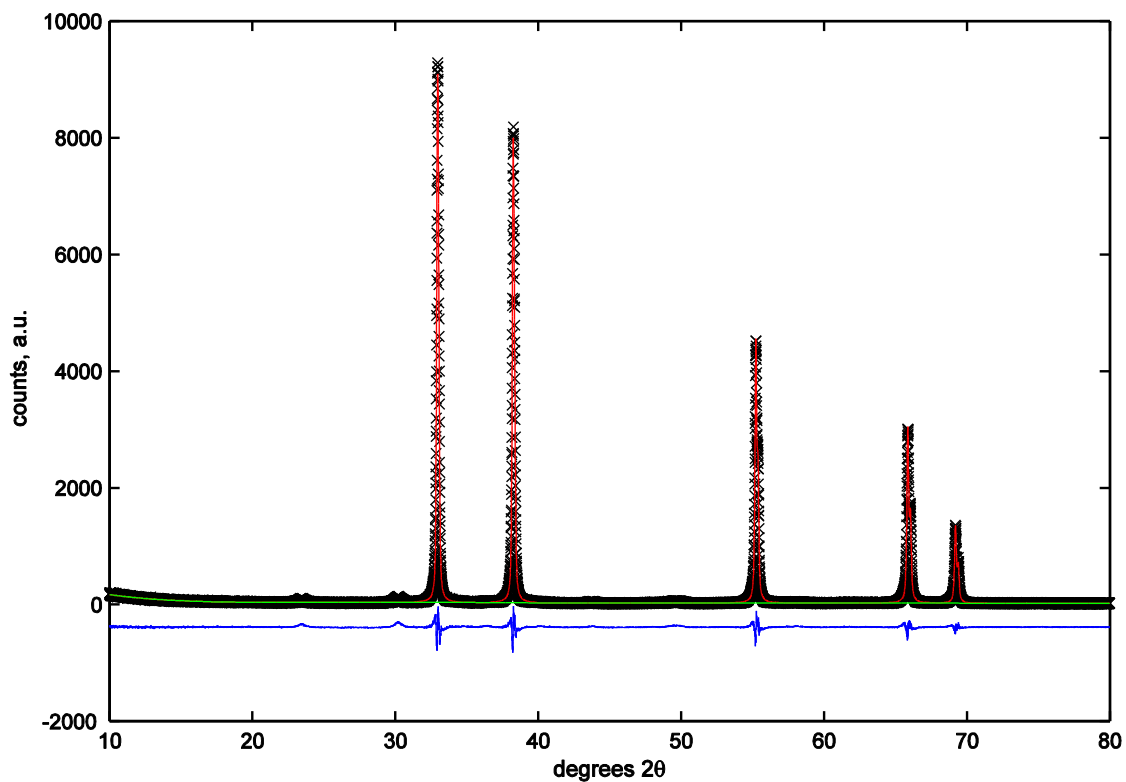


Figure C: Le Bail refinement plot of pure CdO

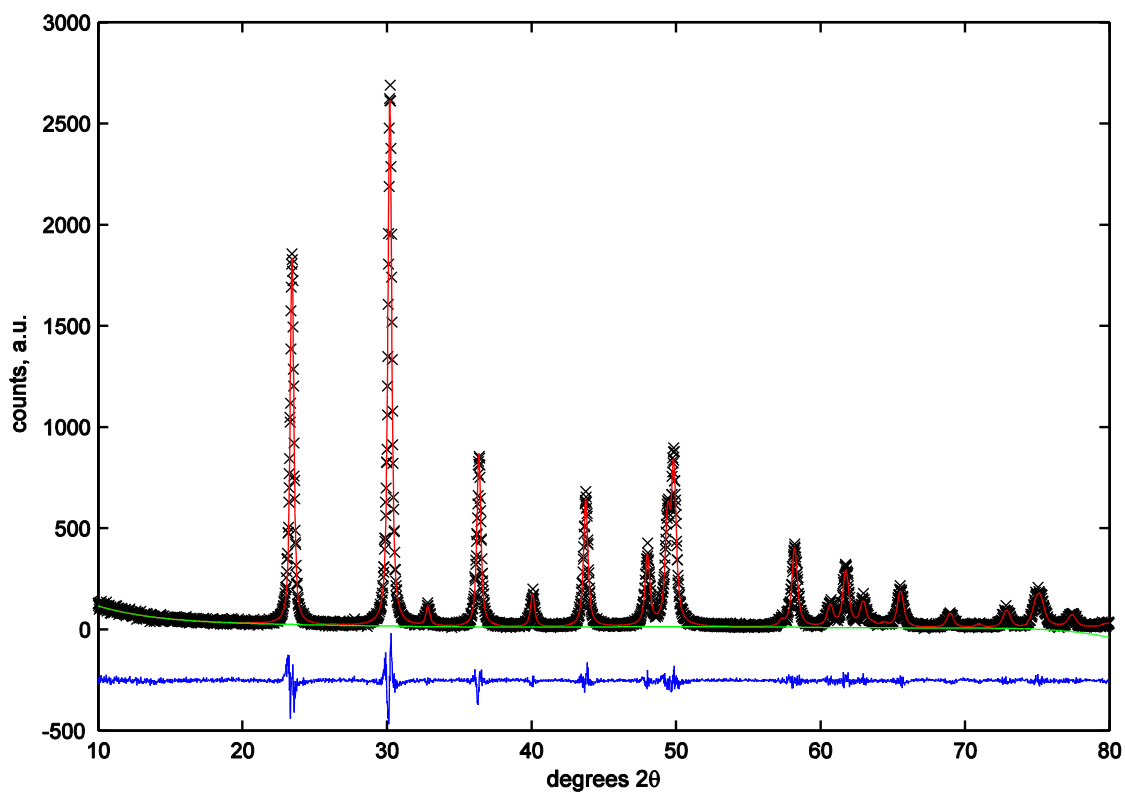


Figure D: Le Bail refinement plot of pure CdCO₃

2.3 Results

Table B: Results of the Le Bail refinement of the laboratory XRD data for cadmium oxide and carbonate

sample	phase	unit cell lengths a = b	unit cell length c	space group
17.5 % NaI calcined 500 °C air 3 h	CdO	4.6994 Å	= a	Fm-3m
pure CdO	CdO	4.6949 Å	= a	Fm-3m
PDF 4+ 2011 entry 04-001-3770	CdO	4.6951 Å	= a	Fm-3m
pure CdCO ₃	CdCO ₃	4.9330 Å	16.3448 Å	R-3c
PDF 4+ 2011 entry 04-014-4823	CdCO ₃	4.9207 Å	16.2968 Å	R-3c

3 EDX results and Powder Diffraction File data

EDX results are given in Figure E to Figure G. The increased iodine content relative to cadmium is evident in Figure F. Table B shows the d-spacings and reciprocal distances for cadmium oxide, Powder Diffraction File entry 04-001-3770.

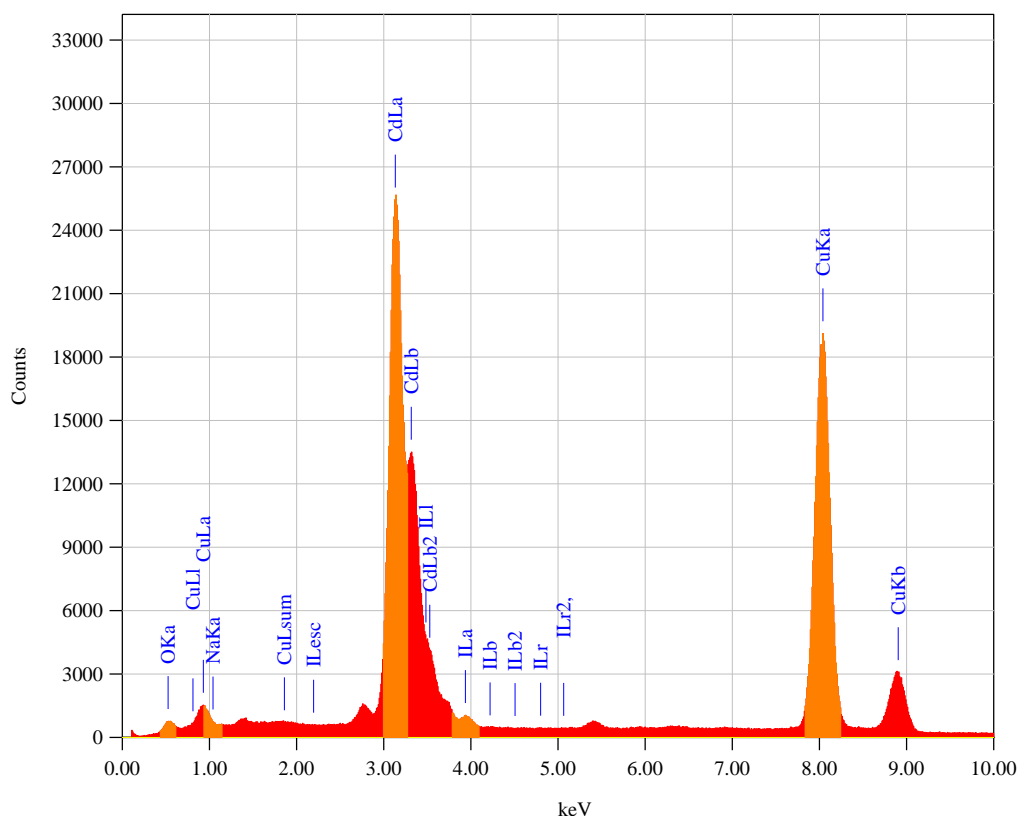


Figure E: EDX spectrum for 'edx 2' label in article.

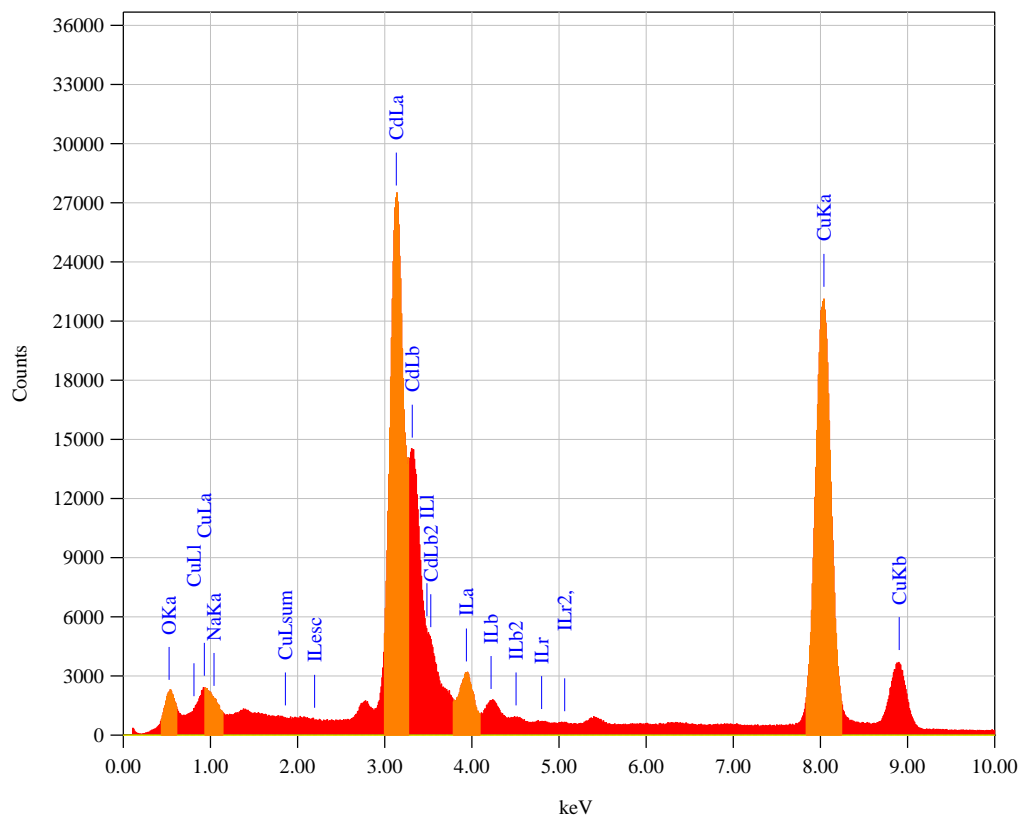


Figure F: EDX spectrum for 'edx 3' label in article.

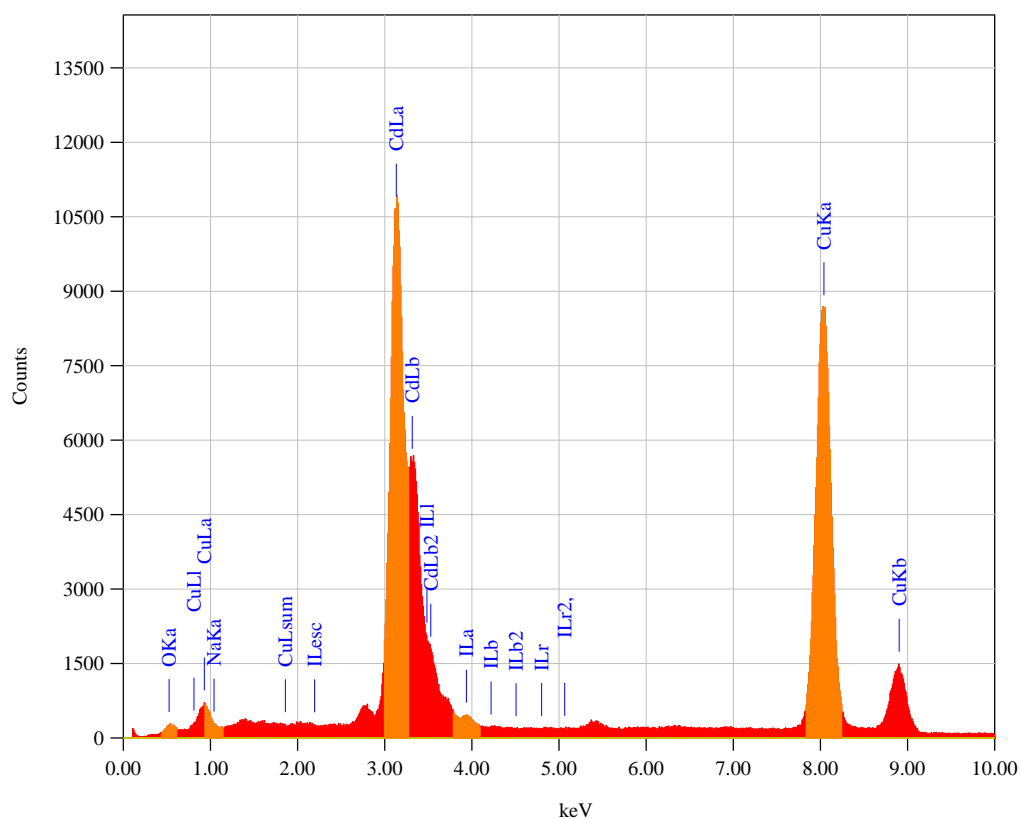


Figure G: EDX spectrum for 'edx 4' label in article.

Table B: Assignment of electron diffraction pattern observations corresponding to label A-K in the article, d-spacing values obtained from Powder Diffraction File entry 04-001-3770 (CdO)

Label	A	B	C	D	E	F	G	H	I	J	K
d-spacing (Å)	2.71	2.35	1.66	1.42	1.36	1.17	1.08	1.05	0.96	0.9	0.83
Reciprocal distance (1/nm)	3.69	4.26	6.02	7.06	7.38	8.52	9.28	9.53	10.43	11.07	12.05
Q (1/Å)	2.32	2.68	3.78	4.44	4.64	5.35	5.83	5.99	6.55	6.96	7.57
h	1	2	2	3	2	4	3	4	4	5	4
k	1	0	2	1	2	0	3	2	2	1	4
l	1	0	0	1	2	0	1	0	2	1	0