

## Supporting information

### Preparation of zirconium oxide powder using zirconium carboxylate precursors

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TABLE S1: The structures of the carboxylic acids used for the preparation of the single precursor ZCs.

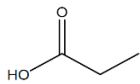
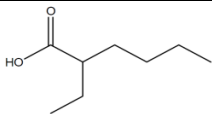
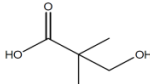
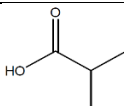
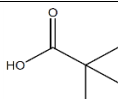
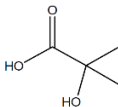
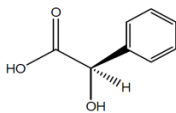
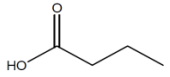
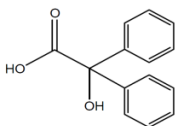
No.	structure	acid	remark
1		propanoic acid	
2		2-ethylhexanoic acid	
3		hydroxypivalic acid	
4		isobutyric acid	
5		pivalic acid	
6		$\alpha$ -hydroxyisobutyric acid	
7		mandelic acid	
8		butyric acid	
9		benzilic acid	Hazmi et al., <i>Science of Advanced Materials</i> , in press.

TABLE S2: Structures and properties of the synthesized ZC complexes used in this study.

sample	(Initial components) ZrOCl <sub>2</sub> ·8H <sub>2</sub> O with :	Calcination to oxide		Oxide temp. (°C) <sup>a</sup>	Product proposed formula <sup>b</sup>	pH	Surface area (m <sup>2</sup> /g)	Product yield (%)	Precursor crystal phase
		ZrO <sub>2</sub> (%)	MW (g/mol)						
<b>ZrAc</b>	Zirconium acetate	58.0	211	590	[Zr <sub>4</sub> O <sub>4</sub> (OH) <sub>3</sub> (OAc) <sub>5</sub> ]4H <sub>2</sub> O	-	0.78	-	Amorphous
<b>Zr-1</b>	Glacial propanoic acid	45.0	273	590	[Zr <sub>4</sub> O <sub>2</sub> (OH) <sub>5</sub> (OAp) <sub>5</sub> Cl <sub>2</sub> ]8H <sub>2</sub> O	0-1	0.56	97	Crystalline
<b>Zr-2</b>	Sodium propionate	48.9	252	590	[Zr <sub>4</sub> O <sub>4</sub> (OH) <sub>3</sub> (OAp) <sub>5</sub> ]7H <sub>2</sub> O	6-7	1.39	95.6	Amorphous
<b>Zr-3</b>	Sodium butyrate	44.6	262	450	[Zr <sub>4</sub> O <sub>4</sub> (OH) <sub>2</sub> (BUT) <sub>6</sub> ]2H <sub>2</sub> O	6	23.5	94	Amorphous
<b>Zr-4</b>	Sodium isobutyrate	42.5	289	450	[Zr <sub>4</sub> O <sub>4</sub> (OH) <sub>2</sub> (ISBUT) <sub>6</sub> ]8H <sub>2</sub> O	6	36.5	100	Amorphous
<b>Zr-5</b>	Ammonium pivalate	40.5	304	380	[Zr <sub>4</sub> O <sub>4.5</sub> (PA) <sub>7</sub> ]5H <sub>2</sub> O	6	297	99.2	Amorphous
<b>Zr-6</b>	Sodium hydroxypivalate	37.7	326	590	[Zr <sub>4</sub> O <sub>5</sub> (HPA) <sub>6</sub> ]8H <sub>2</sub> O	5-6	14.9	64.4	Crystalline
<b>Zr-7</b>	Ammonium 2-ethylhexanoate	47.5	259	470	[Zr <sub>4</sub> O <sub>6</sub> (OH) <sub>2</sub> (EHA) <sub>2</sub> ]7H <sub>2</sub> O	3-4	20.1	74	Amorphous
<b>Zr-8</b>	$\alpha$ -Hydroxyisobutyric acid	27.8	443	590	[Zr <sub>4</sub> (OH) <sub>4</sub> (HIBUTA) <sub>12</sub> ]6H <sub>2</sub> O	0-1	11.3	56	Crystalline
<b>Zr-9</b>	Sodium $\alpha$ -hydroxyisobutyrate	24.4	504	650	[Zr <sub>4</sub> O(OH) <sub>4</sub> (HIBUTA) <sub>10</sub> ]28H <sub>2</sub> O	0-1	6.11	78	Crystalline
<b>Zr-10</b>	Mandelic acid	23.1	532	500	[Zr <sub>4</sub> O(OH) <sub>5</sub> (MA) <sub>9</sub> ]4H <sub>2</sub> O	0-1	13.2	72.2	Crystalline

<sup>a</sup>. The minimum temperatures for the complex conversion of the precursor to zirconium oxide.

<sup>b</sup>. OAc = acetate, OAp = propionate, BUT = butyrate, ISBUT = isobutyrate, PA = pivalate, HPA = hydroxypivalate, EHA = 2-ethylhexanoate, HIBUTA = hydroxyisobutyrate, and MA = mandelate.

TABLE S3: Surface areas and phase composites of ZrO<sub>2</sub> derived from thermal calcinations of ZCs.

Sample <sup>a</sup>	Calcination temperature (°C)	Surface area (m <sup>2</sup> /g)	Phase (%)	
			V <sub>tetragonal</sub>	V <sub>monoclinic</sub>
<b>ZrAc<sup>b</sup></b>	600	4.60	35	65
	720	3.20	8.0	92
	850	0.32	0	100
<b>Zr-1</b>	600	4.10	100	0
	720	0.97	64	36
	850	0.57	-	-
<b>Zr-2</b>	600	2.15	100	0
	720	1.01	59	41
	850	1.77	1.0	99
<b>Zr-3</b>	600	8.30	100	0
	650	10.2	95	5.0
	720	9.56	69	31
	850	7.20	8.0	92
<b>Zr-4</b>	600	6.90	100	0
	650	7.20	94	6.0
	720	5.72	63	37
	850	4.80	0	100
<b>Zr-5</b>	350	14.9	100	0
	500	7.65	100	0
	600	9.30	96	4.0
	720	5.32	69	31
	850	6.30	15	85
<b>Zr-6</b>	600	7.59	85	16
	720	6.64	85	15
	850	6.40	0	100
<b>Zr-7</b>	500	31.6	100	0
	600	16.4	59	41
	720	8.50	28	72
	850	5.30	1.0	99
<b>Zr-8</b>	600	19.8	62	38
	720	8.30	25	75
	850	6.80	0	100
<b>Zr-9</b>	600	3.28	83	17
	720	4.04	19	81
	850	2.70	0	100
<b>Zr-10</b>	500	7.10	100	0
	600	6.97	95	5.0
	720	5.56	65	35
	850	2.87	14	86

a. The specifications correspond to those described in Table S2. b. ZrAc is zirconium (IV) acetate hydroxide.

### Approach to determine the volume fraction

The volume fraction of the tetragonal and monoclinic phases (t-ZrO<sub>2</sub> and m-ZrO<sub>2</sub>, respectively) and the relative ratio of t-ZrO<sub>2</sub> to m-ZrO<sub>2</sub> were determined using the method proposed by Toraya and co-workers [1]. The integrated intensity ratio (X) was calculated by using the area values of the tetragonal characteristic peak at  $2\theta = 30^\circ$  for the (111) reflection and that of the two monoclinic characteristic peaks of the peaks at  $2\theta = 28^\circ$  and  $2\theta = 31^\circ$  for the (11 $\bar{1}$ ) and (111) reflections, respectively, as follows.

$$X_m = \frac{A[(111)]_m + A[m(11\bar{1})]_m}{A[(111)]_t + A[m(111)]_m + A[m(11\bar{1})]_m} \quad (1)$$

$$X_t = \frac{A[(111)]_t}{A[(111)]_t + A[m(111)]_m + A[m(11\bar{1})]_m} \quad (2)$$

where, A and the subscripts (m and t) are areas, monoclinic, and tetragonal, respectively.

The volume fraction (V) was then calculated using the integrated intensity values taking into account the deviation from linearity between the volume fraction and the intensity ratio using the following correction equation [2]:

$$V_m = \frac{1.311X_m}{1 + 0.311X_m} \quad (3)$$

$$V_t = 1 - V_m \quad (4)$$

### References:

- [1] Toraya H, Masahiro M, Somiya S. "Calibration Curve for Quantitative Analysis of the Monoclinic-Tetragonal ZrO<sub>2</sub> System by X-Ray Diffraction," *Journal of the American Ceramic Society*, 1984, 67(6), C119-C121.
- [2] Cuo G-Y, Chen Y-L. "Preparation and characterization of a novel zirconia precursor," *Ceramics International*, 2004, 30, 469-475.