Computational discovery of a large-imine-cage-based porous molecular material and its application in water desalination

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Electronic Supplementary Information (ESI) file

Structure files

Tar archive with structures and tabulated energies can be downloaded from our repository: http://nanoporousmaterials.org/databases/

Figures and Tables

Figure S-1. DFT-refined energy landscape of crystalline phases of CCXL with highlighted positions of the selected 10 phases .

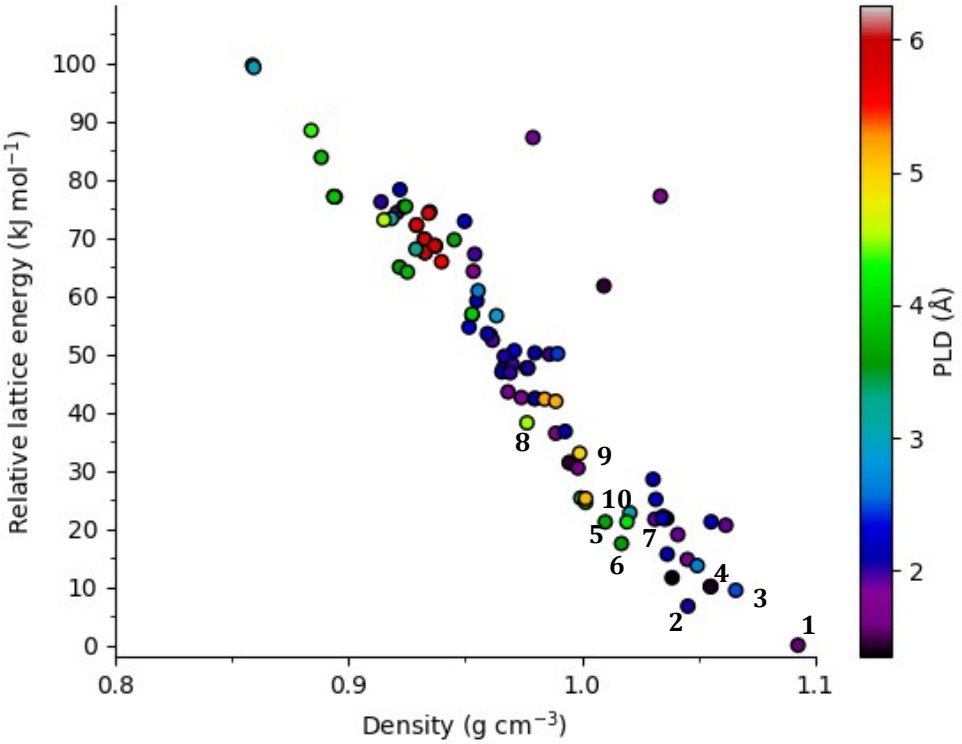

Figure S-2. Illustration of pore landscapes for 10 selected crystalline phases of CCXL. Pore landscapes where obtained for a probe with a diameter of 2.2 Ang. Pore interiors are highlighted in red color.

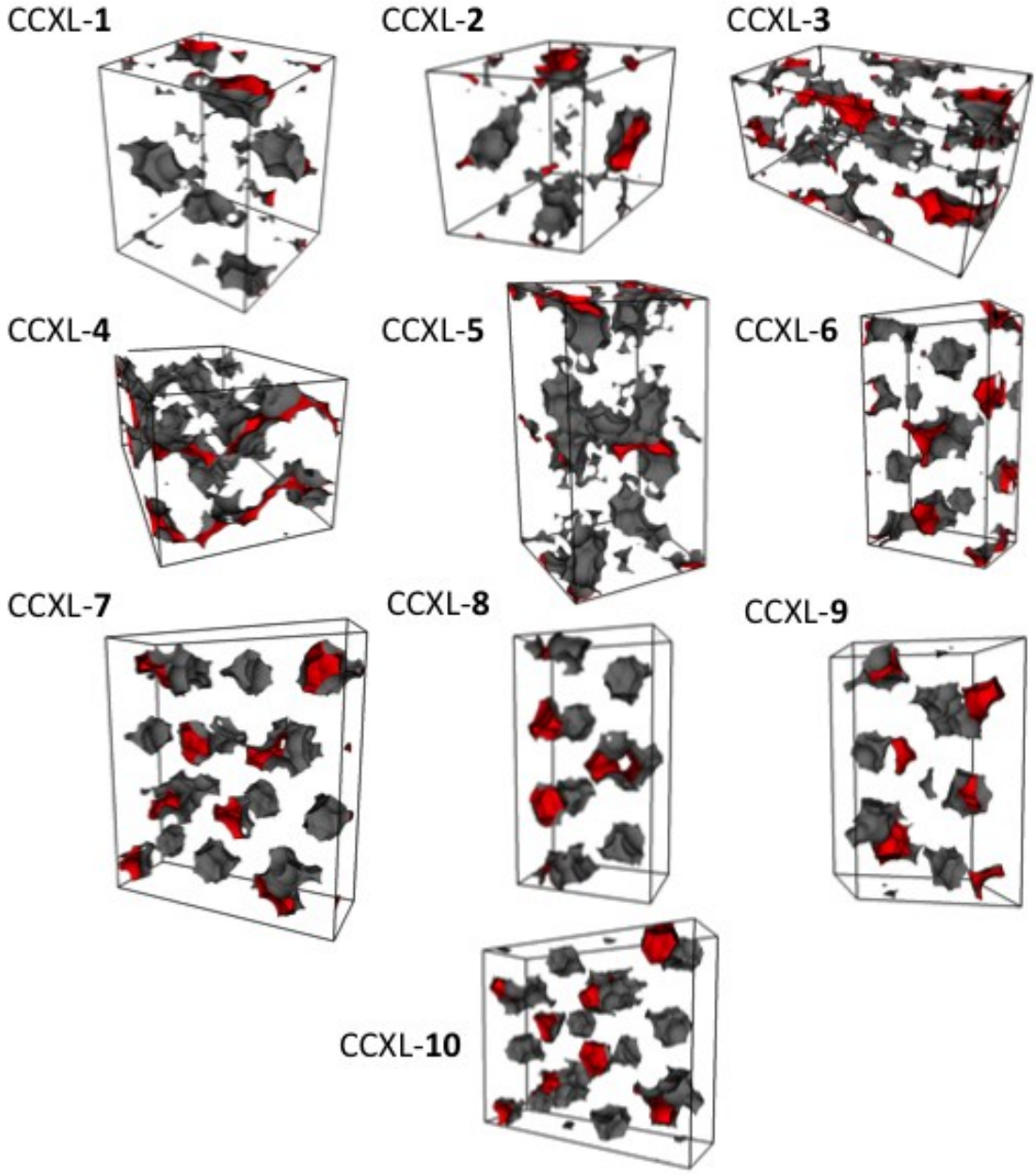

Figure S-3. Energy landscape of crystalline phases of CCXL obtained with classical force-field.

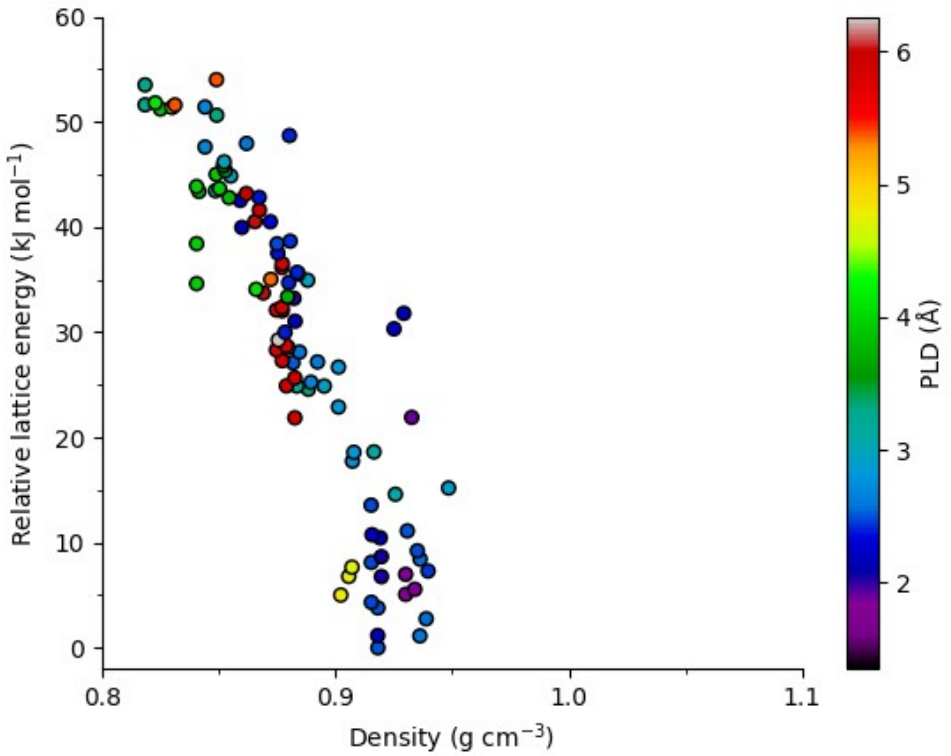

Table S-1. Porosity descriptors for 10 selected crystalline phases of CCXL.

Phase	Density [g/cm³]	Geometrical void fraction (probe r=1.42 Å)	Largest cavity diameter [Å]	Pore limiting diameter [Å]
CCXL-**1**	1.09	0.03	6.35	1.56
CCXL-**2**	1.05	0.04	5.92	2.05
CCXL-**3**	1.07	0.03	6.05	2.49
CCXL-**4**	1.05	0.03	5.91	2.66
CCXL-**5**	1.02	0.04	5.99	3.00
CCXL-**6**	1.02	0.04	6.09	3.63
CCXL-**7**	1.02	0.05	5.99	4.14
CCXL-**8**	0.98	0.06	6.26	4.50
CCXL-**9**	1.00	0.06	6.18	4.98
CCXL-**10**	1.00	0.05	6.14	5.14

Table S-2. Geometry-based characterization of replicas representing amorphous phases of CC3 and CCXL.

Material	Replica ID	Density [g/cm³]	Geometrical void fraction (probe r=1.42 Å)	Largest cavity diameter [Å]	Pore limiting diameter[Å]
CC3	1	0.76	0.12	13.43	3.92
	2	0.77	0.11	12.84	4.11
	3	0.79	0.09	10.82	3.63
	4	0.79	0.09	11.47	3.73
	5	0.77	0.10	11.54	4.36
	6	0.78	0.10	12.92	4.12
	7	0.77	0.10	12.97	4.15
	8	0.74	0.14	23.31	3.79
	9	0.78	0.10	11.73	3.86
	10	0.78	0.10	12.21	3.88
CCXL	1	0.72	0.20	21.86	6.65
	2	0.76	0.17	19.80	5.54
	3	0.75	0.17	15.04	5.66
	4	0.76	0.16	15.84	4.52
	5	0.75	0.17	15.88	6.14
	6	0.74	0.18	16.93	5.60
	7	0.77	0.16	16.86	5.14
	8	0.76	0.17	18.50	5.70
	9	0.76	0.16	15.53	5.66
	10	0.78	0.14	15.65	4.57