

Supplementary Information for

CTAB assisted synthesis of ultra-high aspect ratio $3\text{Mg(OH)}_2\cdot\text{MgCl}_2\cdot8\text{H}_2\text{O}$ nanowires

Lu Gong,^a Zhenying Yao,^a Chunmei Zhu,^a Lan Xiang,^b Xin Lian,^a Bai He,^a Baoyan Fan^c, and Bo Yu*,^a

^a School of Chemistry and Chemical Engineering, Chongqing University of Science and Technology, Chongqing 401331, China

^b Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

^c School of Metallurgy and Materials Engineering, Chongqing University of Science and Technology, Chongqing 401331, China

* Corresponding Author

The FDF file includes:

Figures S1 to S2

Tables S1 to S3

Other supplementary information for this manuscript includes the following.

Movie S1

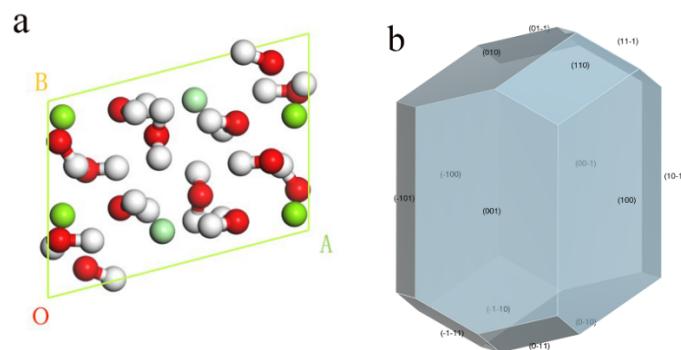


Figure S1. The crystal cell structure of 318MHCH (a) and the morphology of the 318MHCH was determined with the BFDH (b)

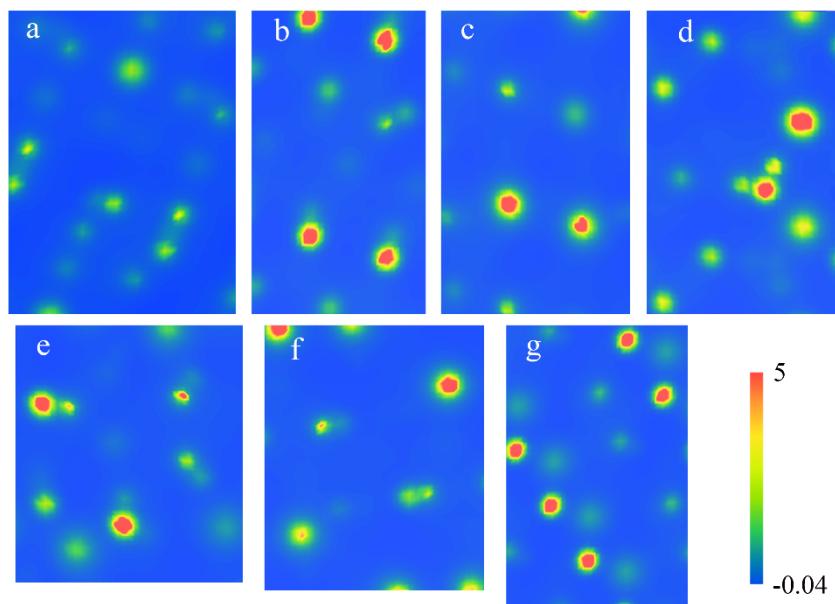


Figure S2. Projection of electrostatic potential on the isosurface of electron density of different crystal surfaces a (-1 0 1), b (0 0 1), c (0 1 -1), d (0 1 0), e (1 1 -1), f (1 1 0), g (1 0 0).

Table S1. SAED spectrum calibration calculation

	pixel distance	Diffraction pattern distance (1/nm)	crystalplane spacing (Å)
ruler	231	5	--
A	164.35	3.55	2.81
B	129.02	2.79	3.58
C	169.61	3.67	2.72

Table. S2 BFDH morphology calculation

<i>hkl</i>	Multiplicity	d_{hkl}	Distance	Total facet	Total facet area
				area	%
(1 0 0)	2	8.122	12.311	1332.924	31.074
(0 0 1)	2	7.129	14.025	1106.606	25.798
(-1 0 1)	2	5.963	16.769	327.490	7.634
(0 1 0)	2	5.935	16.847	745.302	17.375
(1 1 0)	2	5.497	18.189	360.965	8.415
(1 1 -1)	2	5.059	19.763	278.153	6.484
(0 1 -1)	2	4.934	20.263	137.949	3.216

Table. S3 The Interaction energy calculation results

crystal face	Total energy (kcal/mol)	Surface energy (kcal/mol)	CTAB energy (kcal/mol)	Interaction energy (kcal/mol)
(1 0 0)	-5994.983	-6122.958	129.396	-1.421
(0 0 1)	-5882.573	-5983.343	129.396	-28.626
(0 1 0)	-47734.05	-47844.917	129.396	-18.529
(1 1 0)	-46381.205	-46469.097	129.396	-41.504
(-1 0 1)	-11640.695	-11698.479	129.396	-71.612
(1 1 -1)	-38647.970	-38750.13	129.396	-27.236
(0 1 -1)	-9273.166	-9385.52	129.396	-17.042