Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Confinement Induces Stable Calcium Carbonate Formation in Silica Nanopores

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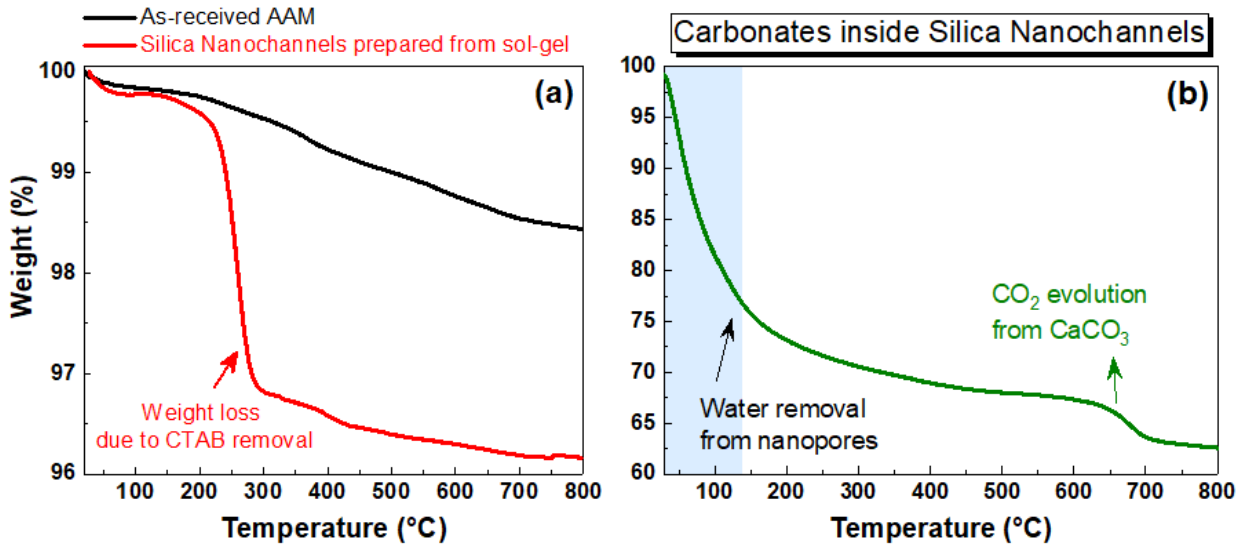

Figure S1. Estimation of weight changes using thermogravimetric analysis (TGA). **(a)** Changes in the weight loss of the as-received anodic alumina membrane (AAM) and silica nanochannels (SNCs) prepared using the sol-gel approach. Weight loss at 250 °C corresponds to CTAB removal from SNCs. **(b)** Changes in the weight associated with the dissociation of calcium carbonate formed in SNCs.

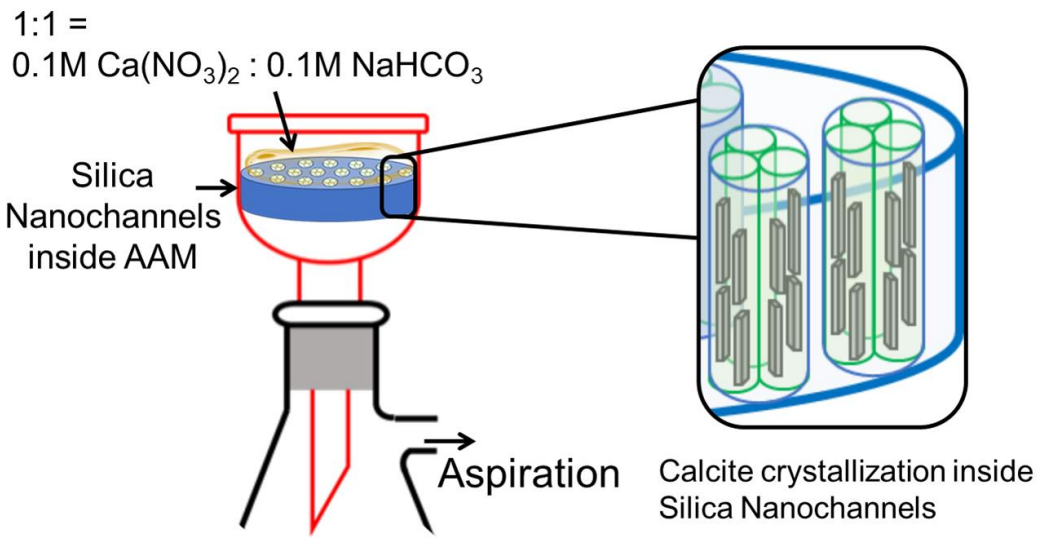

Figure S2. Loading of Ca^{2+} and CO_3^{2-} containing solutions in silica nanochannels. Schematic representation of sample preparation approach for carbonate formation inside silica nanochannels and organization of the formed carbonate crystals.

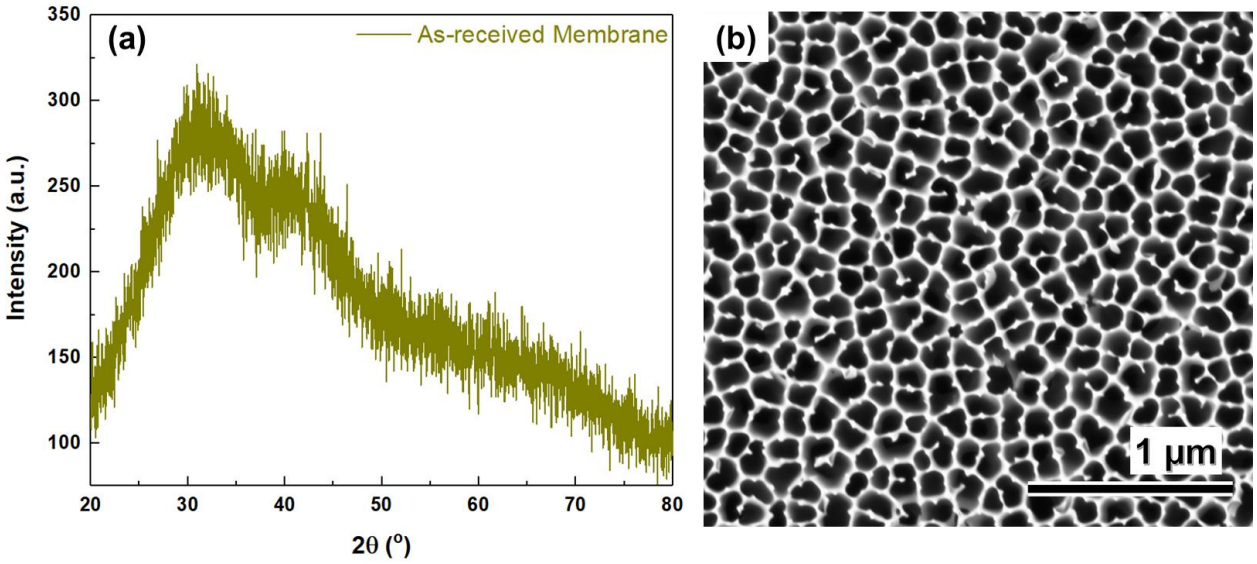

Figure S3. Characterization of the as-received Anodic Alumina Membrane (AAM). **(a)** The amorphous structure of the as-received anodic alumina membrane (AAM) determined using XRD. **(b)** Morphology of as-received membrane imaged using SEM.

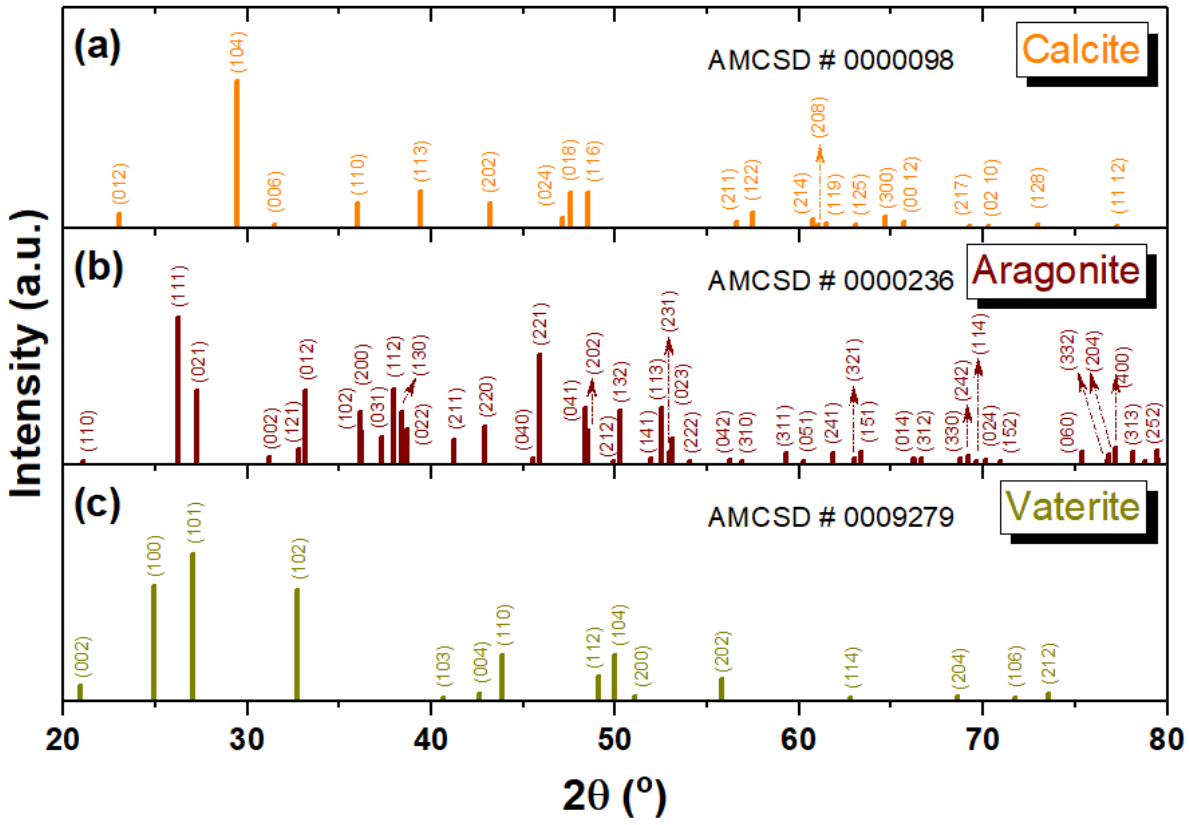

Figure S4. X-ray diffraction (XRD) patterns of different polymorphs of calcium carbonate. Identification of different planes in polymorphs of calcium carbonate ($CaCO_3$) as reported in the American Mineralogist Crystal Structure Database (AMCSD). **(a)** XRD pattern of calcite. **(b)** Aragonite. **(c)** vaterite. The referred AMCSD datasets are also mentioned.

Table S1. The forcefields parameters of the atoms in silica pores, water molecules and ions are obtained from the references listed in Ref. column.

Atom	σ (nm)	ε (kJ/mol)	q (e)	Ref.
Silica				
Si	0.302	7.7006×10^{-6}	2.1000	[1]
O bridging	0.316	0.650190	-1.0500	[1]
O nonbridging	0.316	0.650190	-0.9500	[1]
H	0.000	0.000000	0.4250	[1]
SPCE				
O	0.316	0.6502	-0.82	[2]
H	0.000	0.000	0.41	[2]
Ions				
Ca^{2+}	0.2412	1.88136	2.000	[3]
C (CO_3)	0.356	0.29288	1.420	[3]
O (CO_3)	0.303	0.50208	-1.140	[3]

σ is the finite distance at which the interatomic potential is zero.

ε is the depth of the potential well.

q is the atomic charge.

References

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