Supporting Information

Two-Dimensional Hydrous Silica: Nanosheets and Nanotubes Predicted from First-Principles Simulations

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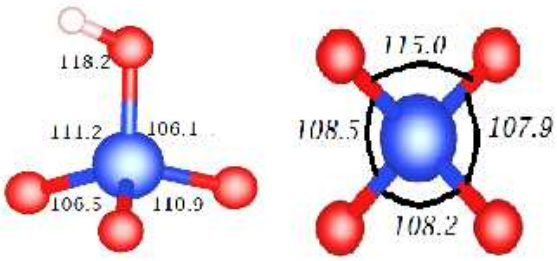
Table S1. Calculated local bonding and total valence electron energies for an isolated water molecule and silicic acid molecule.

	Method	Cube length	Bond lengths and bond angles		Charge	Energy (eV/cell)
A. Water molecule	optB86-vdW	16.5 Å	*d*(O-H):	0.971 Å	$H^{+0.56}{}_2O^{-1.12}$	-13.641
			Angle H-O-H:	104.8°		
B. Silicic acid molecule	optB88-vdW	20.0 Å	*d*(Si-O):	1.643 Å	$Si^{+3.16}(O^{-1.39}H^{+0.60})_4$	-49.480
			d(O-H):	0.968 Å		



(a) (b)

Figure S1. Angles (°) for typical Si-coordination in HSS sheets or/and HSNTs with hexagonal rings (a) and in anhydrous silica sheets or nanotubes (b).

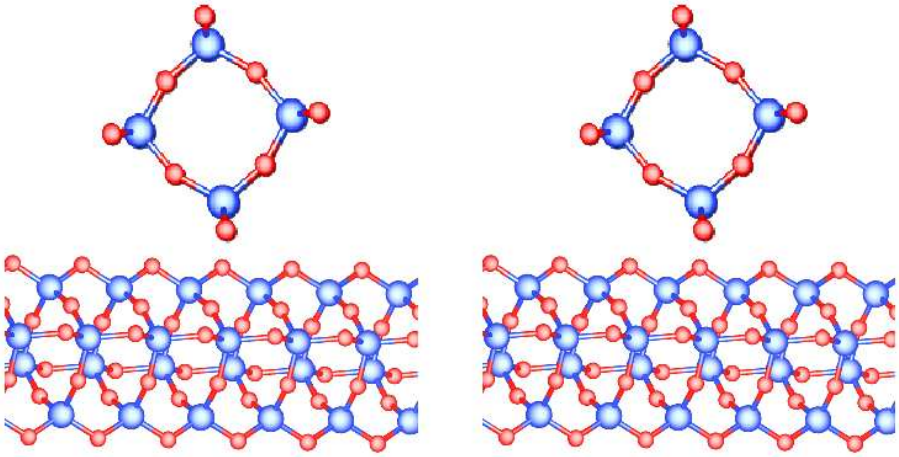
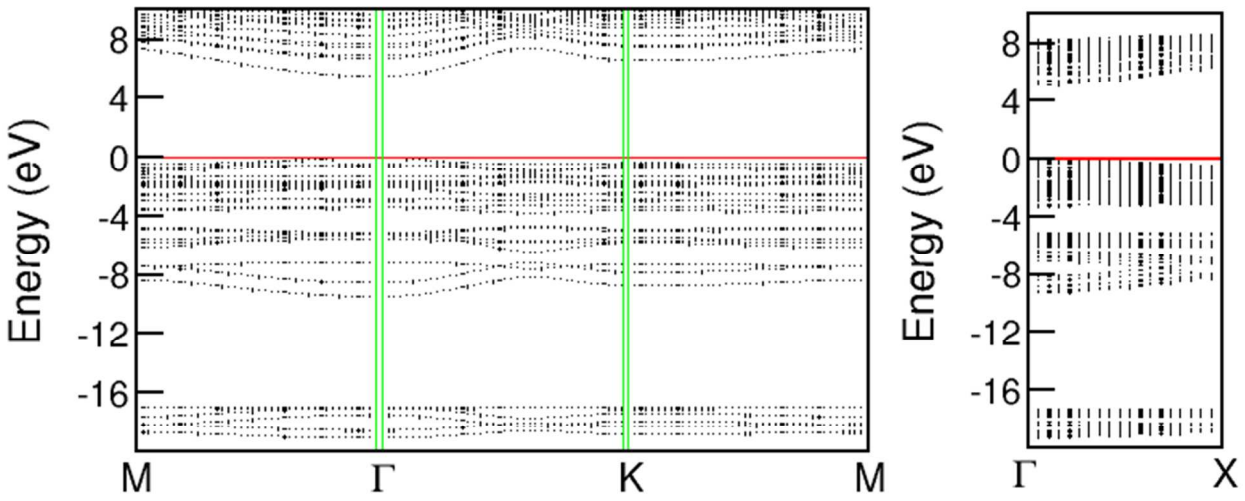


Figure S2. Schematic structural model of an anhydrous silica nanotube with a diameter of about 0.5 nm.



a) b)

Figure S3. Calculated dispersion curves for the 2D anhydrous silica bilayer sheet (see Figure 3a and 3b) and the 1D hydrous silica tube with a quarter of the –(OH) clusters pointing inwards (Figure 1a and 1b).