Structural diversity in sodium doped water trimers: Supplementary Information

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1 Correlation of single point energies

The data shown corresponds to single point energies computed on B3LYP/6-31+G** optimized structures. Zero-point energy corrections are not included. All values mentioned in the main text include the latter corrections, scaled by a factor of 0.963.[1] [1] - G. Rauhut and P. Pulay, J. Phys. Chem. **99**, 3093-3100 (1995).



Figure 1: Correlation of B3LYP/6-31+g** with CCSD(T)/aug-cc-pVTZ single point energies.

2 Spin density plots



Figure 2: Spin density of the lowest minima of classes A-D, obtained at the B3LYP/def2-TZVPP level of theory, cutoff 0.002 Å⁻³.

3 Sample cartesian coordinates

The cartesian coordinates for each lowest-energy minimum of the cluster classes discussed in the main text are given below.

10							
class A							
Na	-1.140202	1.190392	-0.033793				
0	-0.704826	-0.181875	1.720743				
Н	0.264395	-0.202245	1.897614				
H	-1.138044	-0.796816	2.324323				
0	1.990133	0.207383	1.641699				
Н	1.924600	0.875349	0.930126				
Н	2.594302	0.558807	2.307199				
0	1.121187	1.788349	-0.536727				
H	1.313105	1.453306	-1.436380				
Н	1.066015	2.761385	-0.629270				
10							
class B							
Na	-0.922835	-0.441149	0.848685				
0	0.767459	0.288048	2.213688				
Н	1.590801	0.707613	1.915168				
H	1.032135	-0.427038	2.819341				
0	-0.260801	-2.385119	-2.023508				
Н	-0.421006	-2.878139	-1.197395				
Н	0.695270	-2.432538	-2.175527				
0	-1.378310	0.035772	-1.330869				
Н	-2.129207	0.351240	-1.850294				
H	-1.008189	-0.751259	-1.792671				
10							
cla	ss C						
Na	1.406863	0.608673	1.744128				
0	1.904288	1.080392	-0.419223				
H	1.087978	1.146977	-0.977023				
Н	2.626838	0.835997	-1.011280				
0	-0.484194	1.091907	-1.707585				
H	-0.915607	1.914585	-1.968152				
Н	-1.087506	0.641369	-1.072333				
0	-1.946209	-0.166595	0.275375				
Н	-1.491881	-0.006175	1.126300				
Н	-2.100537	-1.120997	0.243474				

10					
class D					
Na	-0.551607	2.593308	2.229892		
0	0.014965	1.714400	0.160625		
Н	0.702919	1.005697	0.076713		
Н	0.091618	2.273923	-0.627002		
0	1.398645	-0.606716	-0.085814		
Н	0.543739	-1.081062	-0.026483		
Н	1.995580	-0.999615	0.562746		
0	-1.349399	-0.904405	-0.031853		
Н	-2.043327	-1.250708	0.543108		
Η	-1.370595	0.065857	0.053966		

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