

Table S7. Totally and partially optimized geometrical parameters of the bridging hydroxyl group Al-OH-Si for the bare zeolite systems ZOH with one to four Al atoms calculated at the PBE-D3 level in periodic model

Zeolite systems ZOH	Total optimization			Partial optimization		
	Al-O ^a	Si-O ^a	AlOSi ^b	Al-O ^a	Si-O ^a	AlOSi ^b
1 Al						
Al1 _{ads}	1.901	1.702	132.9	1.895	1.693	132.5
Al2 _{ads}	1.884	1.699	135.4	1.867	1.691	136.2
Al3 _{ads}	1.912	1.697	140.6	1.898	1.688	139.8
Al4 _{ads}	1.899	1.699	132.3	1.888	1.692	132.4
2 Al						
Al1 _{ads} Al2	1.900	1.701	133.2	1.892	1.694	132.6
Al1 _{ads} Al3	1.907	1.705	133.1	1.893	1.697	132.3
Al1 _{ads} Al4	1.902	1.701	133.2	1.896	1.694	132.8
Al2 _{ads} Al1	1.880	1.701	135.2	1.868	1.692	135.9
Al2 _{ads} Al3	1.876	1.705	135.5	1.861	1.695	136.0
Al2 _{ads} Al4	1.882	1.703	135.8	1.865	1.693	135.3
Al3 _{ads} Al1	1.914	1.699	141.1	1.897	1.693	140.5
Al3 _{ads} Al2	1.903	1.703	139.4	1.887	1.698	140.1
Al3 _{ads} Al4	1.913	1.696	140.3	1.903	1.689	140.1
Al4 _{ads} Al1	1.897	1.699	132.4	1.893	1.693	132.7
Al4 _{ads} Al2	1.893	1.702	131.3	1.891	1.697	131.8
Al4 _{ads} Al3	1.899	1.697	132.7	1.889	1.692	133.1
3 Al						
Al1 _{ads} Al2Al3	1.906	1.707	133.8	1.891	1.698	132.6
Al1 _{ads} Al2Al4	1.902	1.703	138.7	1.891	1.694	133.0
Al1 _{ads} Al3Al4	1.905	1.707	133.6	1.897	1.696	132.8
Al2 _{ads} Al1Al3	1.876	1.708	136.1	1.860	1.697	136.3
Al2 _{ads} Al1Al4	1.880	1.706	136.2	1.861	1.695	135.8
Al2 _{ads} Al3Al4	1.876	1.709	135.8	1.858	1.699	136.3
Al3 _{ads} Al1Al2	1.902	1.706	139.9	1.885	1.702	140.7
Al3 _{ads} Al1Al4	1.909	1.699	139.9	1.897	1.693	140.6
Al3 _{ads} Al2Al4	1.903	1.702	139.2	1.890	1.698	140.2
Al4 _{ads} Al1Al2	1.896	1.701	132.1	1.890	1.697	132.2
Al4 _{ads} Al1Al3	1.898	1.699	133.2	1.893	1.692	133.2
Al4 _{ads} Al2Al3	1.893	1.700	131.5	1.889	1.696	132.5
4 Al						
Al1 _{ads} Al2Al3Al4	1.901	1.707	133.9	1.892	1.697	133.2
Al2 _{ads} Al1Al3Al4	1.876	1.710	136.6	1.867	1.700	136.5
Al3 _{ads} Al1Al2Al4	1.899	1.704	139.7	1.887	1.707	140.8
Al4 _{ads} Al1Al2Al3	1.892	1.700	131.6	1.891	1.695	132.7

^aIn Å; ^bIn deg.