Table S8. Totally and Partially optimized geometrical parameters of the bridging hydroxyl group Al-O-Si for PYH^+/ZO^- adsorption complexes with one to four Al atoms calculated at the PBE-D3 level in periodic model

PYH^+/ZO^- Adsorption complexes	Total optimization			Partial optimization		
	Al-O[a]	Si-O[a]	AlOSi[b]	Al-O[a]	Si-O[a]	AlOSi[b]
1 Al						
$Al1_{ads}$	1.782	1.612	130.5	1.774	1.609	129.4
$Al2_{ads}$	1.767	1.605	137.7	1.756	1.601	137.8
$Al3_{ads}$	1.788	1.610	142.0	1.778	1.603	141.9
$Al4_{ads}$	1.786	1.612	129.8	1.772	1.605	130.4
2 Al						
$Al1_{ads}Al2$	1.782	1.612	131.4	1.772	1.609	129.8
$Al1_{ads}Al3$	1.782	1.614	131.2	1.773	1.611	129.8
$Al1_{ads}Al4$	1.781	1.612	130.7	1.773	1.608	129.6
$Al2_{ads}Al1$	1.773	1.611	136.6	1.760	1.604	136.5
$Al2_{ads}Al3$	1.763	1.610	137.4	1.754	1.607	137.2
$Al2_{ads}Al4$	1.769	1.608	136.7	1.754	1.604	136.8
$Al3_{ads}Al1$	1.789	1.612	142.5	1.777	1.605	141.7
$Al3_{ads}Al2$	1.779	1.614	142.2	1.769	1.09	139.6
$Al3_{ads}Al4$	1.787	1.609	140.9	1.774	1.602	142.0
$Al4_{ads}Al1$	1.785	1.612	130.0	1.771	1.606	130.2
$Al4_{ads}Al2$	1.782	1.615	122.7	1.773	1.609	130.2
$Al4_{ads}Al3$	1.783	1.612	130.8	1.773	1.606	130.4
3 Al						
$Al1_{ads}Al2Al3$	1.787	1.616	131.5	1.777	1.613	130.0
$Al1_{ads}Al2Al4$	1.784	1.614	130.3	1.772	1.609	130.3
$Al1_{ads}Al3Al4$	1.784	1.616	131.5	1.773	1.611	129.5
$Al2_{ads}Al1Al3$	1.768	1.614	138.7	1.752	1.608	135.9
$Al2_{ads}Al1Al4$	1.769	1.612	137.8	1.757	1.606	136.5
$Al2_{ads}Al3Al4$	1.762	1.613	137.7	1.749	1.609	136.9
$Al3_{ads}Al1Al2$	1.784	1.618	139.6	1.768	1.612	139.1
$Al3_{ads}Al1Al4$	1.787	1.611	141.1	1.776	1.606	141.7
$Al3_{ads}Al2Al4$	1.782	1.615	138.3	1.769	1.608	141.8
$Al4_{ads}Al1Al2$	1.782	1.614	130.2	1.771	1.609	130.4
$Al4_{ads}Al1Al3$	1.781	1.611	131.4	1.773	1.606	130.4
$Al4_{ads}Al2Al3$	1.780	1.615	130.0	1.774	1.610	130.3
4 Al						
$Al1_{ads}Al2Al3Al4$	1.785	1.616	132.2	1.773	1.612	130.2
$Al2_{ads}Al1Al3Al4$	1.768	1.615	134.9	1.751	1.611	136.9
$Al3_{ads}Al1Al2Al4$	1.780	1.615	141.5	1.768	1.610	141.8
$Al4_{ads}Al1Al2Al3$	1.786	1.617	128.9	1.775	1.610	130.5

[a]In Å; [b]In deg.