Table S13 Relative Total Electronic Energies E_{rel} (in kcal/mol) of PYH^+/ZO^- Adsorption Complexes of Different Si/Al Ratios and Al Distributions Determined at the PBE-D3/6-31+G(d) Optimized Geometries and Corresponding Single Point E_{rel} Determined at the PBE-D3/6-31++G(2d,2p) and M06-2X-D3/6-31++G(2d,2p) Levels in Cluster Model.

PYH^+/ZO^- Adsorption Complexes	E_{rel}		
	PBE-D3/6-31+G(d)	PBE-D3/6-31++G(2d,2p)	M06-2X-D3/6-31++G(2d,2p)
(31Si,1Al)			
$Al1_{ads}$	2.2	2.3	0.7
$Al2_{ads}$	5.0	5.9	5.3
$Al3_{ads}$	0.0	0.0	0.0
$Al4_{ads}$	15.9	15.8	10.2
(30Si,2Al)			
$Al1_{ads}Al2$	4.8	5.2	5.2
$Al1_{ads}Al3$	9.8	10.6	11.0
$Al1_{ads}Al4$	8.0	8.4	7.8
$Al2_{ads}Al1$	8.3	9.5	9.4
$Al2_{ads}Al3$	9.3	10.6	12.0
$Al2_{ads}Al4$	7.9	8.7	9.4
$Al3_{ads}Al1$	0.0	0.0	0.0
$Al3_{ads}Al2$	4.4	4.8	4.1
$Al3_{ads}Al4$	5.8	6.2	7.3
$Al4_{ads}Al1$	16.6	16.8	11.7
$Al4_{ads}Al2$	24.5	23.7	18.0
$Al4_{ads}Al3$	17.2	17.1	13.6
(29Si,3Al)			
$Al1_{ads}Al2Al3$	7.1	6.9	10.0
$Al1_{ads}Al2Al4$	4.3	4.3	5.0
$Al1_{ads}Al3Al4$	8.9	9.1	11.2
$Al2_{ads}Al1Al3$	7.0	8.0	9.2
$Al2_{ads}Al1Al4$	6.1	6.4	8.2
$Al2_{ads}Al3Al4$	7.3	8.0	10.7
$Al3_{ads}Al1Al2$	0.0	0.0	0.0
$Al3_{ads}Al1Al4$	0.7	0.7	1.7
$Al3_{ads}Al2Al4$	4.8	4.6	4.8
$Al4_{ads}Al1Al2$	19.2	18.2	13.1
$Al4_{ads}Al1Al3$	12.6	12.2	9.4
$Al4_{ads}Al2Al3$	20.4	19.0	15.5
(28Si,4Al)			
$Al1_{ads}Al2Al3Al4$	6.1	5.8	8.6
$Al2_{ads}Al1Al3Al4$	2.0	3.0	4.6
$Al3_{ads}Al1Al2Al4$	0.0	0.0	0.0
$Al4_{ads}Al1Al2Al3$	14.8	13.8	10.0