

Table S14 Average Relative Total Electronic Energies E_{rel} (in kcal/mol) of PYH^+/ZO^- 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)
Intersection Region			
(31Si,1Al)	3.6	4.1	3.0
(30Si,2Al)	7.3	8.0	8.3
(29Si,3Al)	5.8	6.0	7.6
(28Si,4Al)	4.1	4.4	6.6
Narrow Region			
(31Si,1Al)	15.9	15.8	10.2
(30Si,2Al)	19.4	19.2	14.4
(29Si,3Al)	17.4	16.5	12.7
(28Si,4Al)	14.8	13.8	10.0