

Table S15 BSSE Corrected Adsorption Energies E_{ads} (in kcal/mol) and Corresponding Dispersive Energy Contributions (E_{disp}) (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_{ads} 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_{ads} (E_{disp})		
	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)			
Al1 _{ads}	-45.4 (-15.0)	-44.9 (-14.5)	-38.1 (-7.7)
Al2 _{ads}	-45.8 (-14.5)	-44.2 (-12.9)	-36.1 (-4.8)
Al3 _{ads}	-48.8 (-15.2)	-48.5 (-14.9)	-42.0 (-8.4)
(30Si,2Al)			
Al1 _{ads} Al2	-46.0 (-14.8)	-45.5 (-14.3)	-37.5 (-6.3)
Al1 _{ads} Al3	-39.8 (14.9)	-38.7 (-13.9)	-32.5 (-7.7)
Al1 _{ads} Al4	-44.4 (-14.9)	-43.8 (-14.3)	-36.9 (-7.4)
Al2 _{ads} Al1	-42.9 (-14.0)	-41.1 (-12.2)	-33.2 (-4.3)
Al2 _{ads} Al3	-43.7 (14.9)	-42.2 (-13.4)	-34.5 (-5.7)
Al2 _{ads} Al4	-46.7 (-14.2)	-45.0 (-12.5)	-36.6 (-4.1)
Al3 _{ads} Al1	-49.1 (-15.8)	-48.9 (-15.5)	-43.1 (-9.7)
Al3 _{ads} Al2	-48.5 (15.2)	-47.6 (-14.3)	-42.0 (-8.7)
Al3 _{ads} Al4	-47.1 (-15.0)	-46.5 (-14.4)	-39.5 (-7.4)
(29Si,3Al)			
Al1 _{ads} Al2Al3	-41.0 (-14.7)	-40.8 (-14.6)	-32.4 (-6.2)
Al1 _{ads} Al2Al4	-45.0 (-14.7)	-44.4 (-14.1)	-36.6 (-6.3)
Al1 _{ads} Al3Al4	-39.8 (-15.0)	-39.3 (-14.5)	-31.9 (-7.1)
Al2 _{ads} Al1Al3	-41.2 (-13.4)	-40.2 (-12.4)	-33.5 (-5.7)
Al2 _{ads} Al1Al4	-43.5 (-14.2)	-42.3 (-12.9)	-33.4 (-4.0)
Al2 _{ads} Al3Al4	-43.6 (-14.5)	-41.9 (-12.8)	-33.6 (-4.5)
Al3 _{ads} Al1Al2	-47.6 (-15.4)	-46.7 (-14.5)	-41.3 (-9.1)
Al3 _{ads} Al1Al4	-47.7 (-15.6)	-47.1 (-14.9)	-40.8 (-8.7)
Al3 _{ads} Al2Al4	-45.9 (-15.0)	-44.8 (-14.0)	-39.0 (-8.2)
(28Si,4Al)			
Al1 _{ads} Al2Al3Al4	-39.7 (-14.5)	-39.6 (-14.4)	-31.9 (-6.7)
Al2 _{ads} Al1Al3Al4	-43.9 (-14.3)	-42.2 (-12.7)	-36.2 (-6.7)
Al3 _{ads} Al1Al2Al4	-45.4 (-15.2)	-44.4 (-14.2)	-37.4 (-7.2)
Narrow Region			
(31Si,1Al)			
Al4 _{ads}	-31.8 (-20.1)	-31.5 (-19.8)	-29.1 (-17.4)
(30Si,2Al)			
Al4 _{ads} Al1	-32.0 (-20.0)	-31.5 (-19.5)	-29.1 (-17.1)
Al4 _{ads} Al2	-26.3 (-20.3)	-26.1 (-20.0)	-24.1 (-18.0)
Al4 _{ads} Al3	-34.0 (-20.8)	-32.5 (-20.0)	-30.0 (-17.5)
(29Si,3Al)			
Al4 _{ads} Al1Al2	-26.5 (-20.2)	-26.2 (-20.0)	-24.3 (-18.1)
Al4 _{ads} Al1Al3	-32.8 (-20.1)	-32.3 (-19.6)	-29.8 (-17.1)
Al4 _{ads} Al2Al3	-27.2 (-20.4)	-27.2 (-20.3)	-25.1 (-18.2)
(28Si,4Al)			
Al4 _{ads} Al1Al2Al3	-27.3 (-20.3)	-27.3 (-20.3)	-25.2 (-18.2)