Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Table S5. Optimized Intermolecular Geometrical Parameters of PYH^+/ZO^- Adsorption Complexes with Three Al Atoms Calculated at the PBE and PBE-D3 (in brackets) Levels in Cluster and Periodic Models.

PYH^+/ZO^- Adsorption Complexes	Cluster Model (32T)				Periodic Model (96T)			
	O…H[a]	N–H[a]	O…H–N[b]	α[bc]	O…H[a]	N–H[a]	O…H–N[b]	α[bc]
$Al1_{ads}Al2Al3$	1.549(1.549)	1.094(1.093)	176.0(176.7)	31.4(33.7)	1.691(1.659)	1.070(1.072)	175.8(176.0)	25.7(26.0)
$Al1_{ads}Al2Al4$	1.598(1.598)	1.081(1.080)	175.6(176.3)	38.3(40.2)	1.702(1.670)	1.065(1.067)	176.2(171.6)	26.3(24.3)
$Al1_{ads}Al3Al4$	1.550(1.563)	1.090(1.088)	175.9(174.2)	31.8(45.8)	1.671(1.708)	1.069(1.065)	172.9(174.1)	35.9(35.9)
$Al2_{ads}Al1Al3$	1.595(1.592)	1.080(1.080)	168.0(167.4)	70.6(71.4)	1.634(1.647)	1.073(1.072)	165.8(166.9)	76.9(75.4)
$Al2_{ads}Al1Al4$	1.581(1.580)	1.082(1.082)	168.7(168.7)	79.8(77.4)	1.636(1.617)	1.073(1.074)	169.2(171.3)	77.1(72.7)
$Al2_{ads}Al3Al4$	1.604(1.596)	1.078(1.079)	169.5(170.2)	69.4(64.0)	1.622(1.635)	1.072(1.071)	172.8(172.5)	68.7(68.6)
$Al3_{ads}Al1Al2$	1.710(1.704)	1.068(1.067)	177.9(177.2)	30.6(30.5)	1.640(1.613)	1.072(1.072)	175.2(170.2)	65.0(69.8)
$Al3_{ads}Al1Al4$	1.651(1.644)	1.073(1.072)	174.1(171.9)	62.3(71.5)	1.705(1.589)	1.062(1.073)	165.7(173.3)	67.7(72.8)
$Al3_{ads}Al2Al4$	1.670(1.661)	1.070(1.070)	173.6(173.6)	47.5(48.7)	1.676(1.574)	1.065(1.074)	169.2(170.9)	74.8(75.7)
$Al4_{ads}Al1Al2$	1.627(1.629)	1.077(1.077)	158.1(160.2)	63.1(60.4)	1.713(1.722)	1.060(1.057)	150.8(149.7)	68.4(67.6)
$Al4_{ads}Al1Al3$	1.666(1.666)	1.070(1.070)	159.6(161.0)	62.2(59.5)	1.736(1.730)	1.055(1.055)	150.2(149.3)	71.4(70.7)
$Al4_{ads}Al2Al3$	1.624(1.630)	1.077(1.077)	158.2(160.6)	63.8(60.3)	1.692(1.699)	1.062(1.060)	151.7(150.5)	70.2(69.7)

[a]In Å; [b]In deg [c]Angle between the straight channel axis and the vector normal to the PY plane.