Table S6. Optimized Intermolecular Geometrical Parameters of PYH^+/ZO^- Adsorption Complexes with Four 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]
$Al1_{ads}Al2Al3Al4$	1.536(1.534)	1.097(1.096)	175.9(176.5)	30.4(32.9)	1.658(1.652)	1.072(1.072)	175.1(175.0)	23.5(22.5)
$Al2_{ads}Al1Al3Al4$	1.614(1.610)	1.077(1.078)	170.0(171.1)	53.6(54.1)	1.660(1.607)	1.071(1.079)	163.3(169.5)	78.7(72.4)
$Al3_{ads}Al1Al2Al4$	1.691(1.676)	1.071(1.072)	179.1(178.4)	27.2(27.3)	1.652(1.652)	1.071(1.085)	169.9(169.7)	65.9(71.3)
$Al4_{ads}Al1Al2Al3$	1.622(1.626)	1.077(1.077)	158.5(161.1)	59.5(59.5)	1.698(1.688)	1.062(1.061)	151.6(150.9)	70.4(69.7)

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