Supplementary Information (SI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2025

Table S3. Optimized Intermolecular Geometrical Parameters of PYH^+/ZO^- Adsorption Complexes with One Al Atom 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]
$Al1_{ads}$	1.629(1.651)	1.073(1.070)	173.2(170.1)	38.8(45.8)	1.724(1.731)	1.060(1.059)	177.1(173.6)	34.4(38.4)
$Al2_{ads}$	1.592(1.593)	1.076(1.075)	171.9(170.8)	73.1(69.1)	1.589(1.601)	1.074(1.072)	174.4(173.8)	69.5(68.5)
$Al3_{ads}$	1.673(1.676)	1.067(1.065)	178.4(174.9)	77.7(76.9)	1.597(1.581)	1.071(1.071)	174.7(174.8)	75.6(75.6)
$Al4_{ads}$	1.675(1.669)	1.069(1.070)	158.4(159.6)	63.3(61.6)	1.757(1.763)	1.053(1.051)	147.7(147.3)	69.5(69.7)

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