Supporting information for

Behaviour of Surface Hydroxide Groups of Exfoliated Kaolinite in Gas Phase and during Water Adsorption

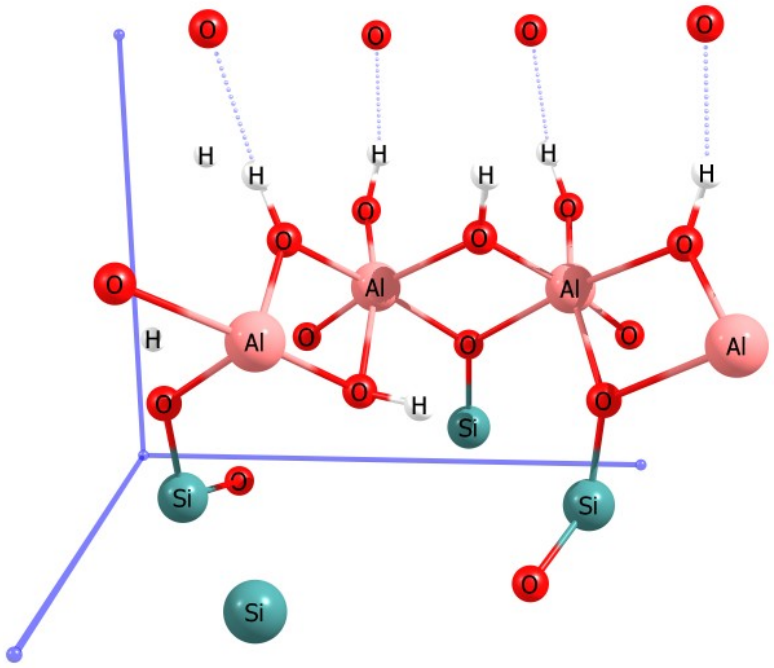
Attila Táborosi and Róbert K. Szilágyi*

Department of Environmental Engineering, Faculty of Engineering, University of Pannonia, PO Box 10, Veszprém, H-8201 HUNGARY
and
Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT 59717 U.S.A.
E-mail: szilagyi@montana.edu

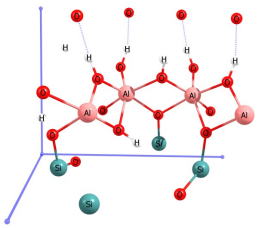
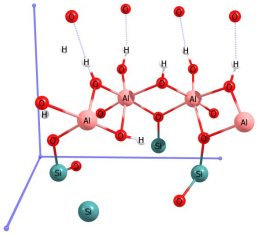
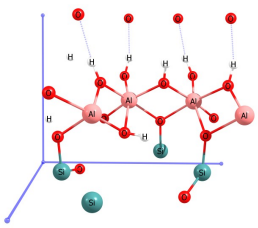
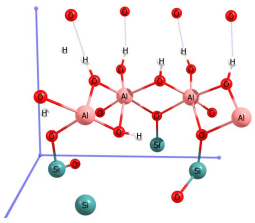
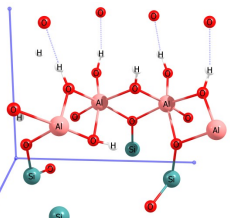
Periodic Models (PBC)

Crystalline Phase - 1x1x1 unit cell

- initial structure

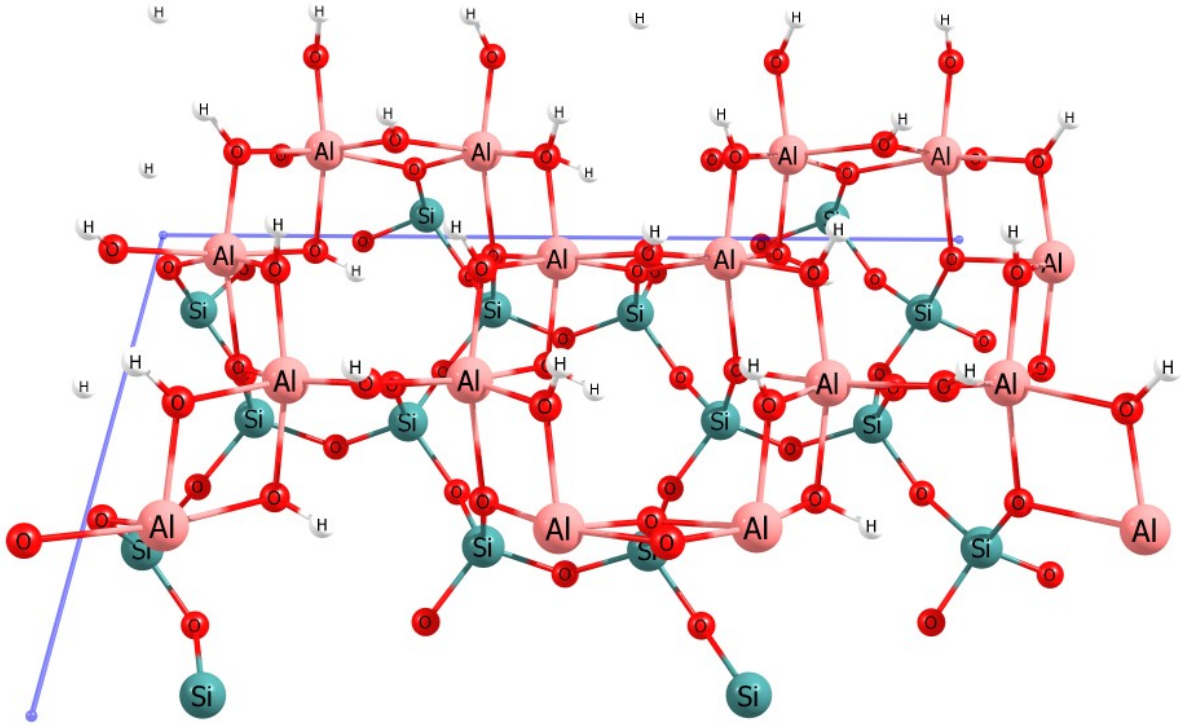


- optimized at functional (rows) and basis set (columns) level of theory

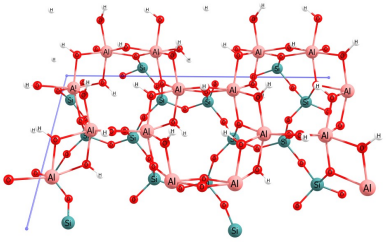
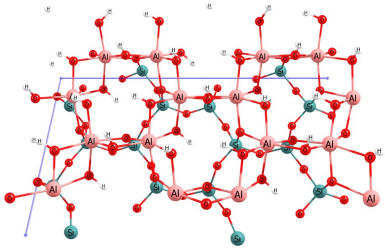
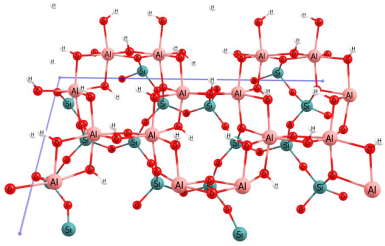
	SDD	6-31G(d)	def2-TZVP
PW91			
BP86			

Slab models - 2x2 unit cell

- initial structure

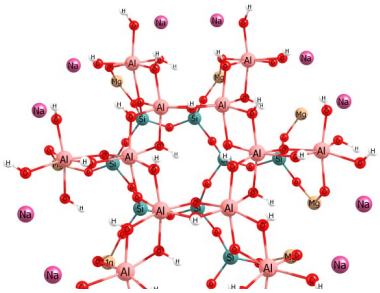


- optimized at functional (rows) and basis set (columns) level of theory

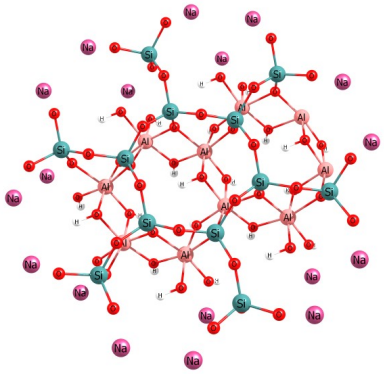
	SDD	6-31G(d)	def2-TZVP
PW91			
BP86			

Molecular Cluster Models

Validation of the Level of Theory



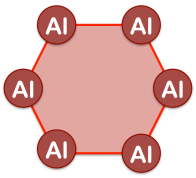
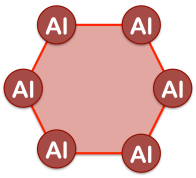
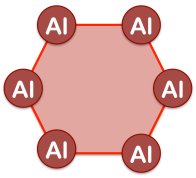
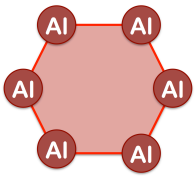
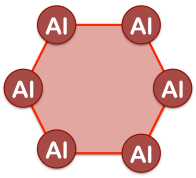
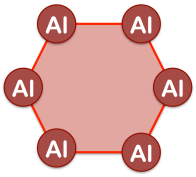
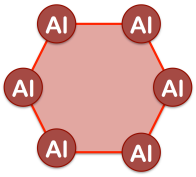
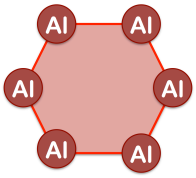
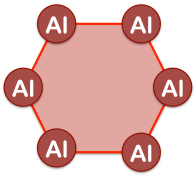
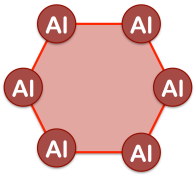
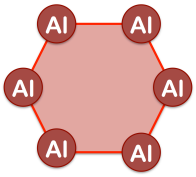
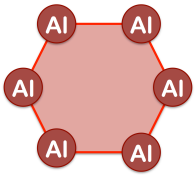
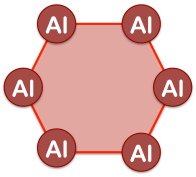
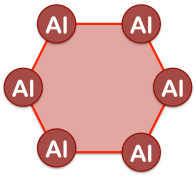
- initial Al-honeycomb and Si-honeycomb



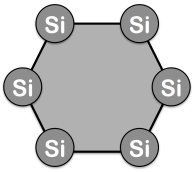
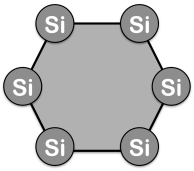
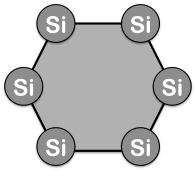
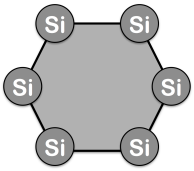
- optimized at functional (rows) and basis set (columns) level of theory

for the [6Al-6(*s*-HO^-)]-honeycomb

molecules/6Al-6OH_HF-LANL2DZ.xyz molecules/6Al-6OH_HF-SDD.xyz

	LANL2DZ	SDD	6-31G(d)	def2-TZV	def2-TZVP
HF					
HF-LYP					
PW91					
BP86					
BLYP					
B3LYP					
+PCM +dispersion +fine grid					

for the [6Si-6(*b*-O^{2-})]-honeycomb

	LANL2DZ	SDD	6-31G(d)	def2-TZV	def2-TZVP
HF					
PW91					
B3LYP					

Position and Orientation of the Surface Exposed *s*-HO^{-}) and *b*-O^{2-} Groups for Nanoclays

Octahedral Layer - [6Al-6(*s*-HO^{-})] honeycomb

ideal clean surface in the absence of solvent media

initial 8 structures for all possible orientations of the surface hydroxide groups in the order of alpha, beta, beta (clockwise)

NEE
ENN
NEN
NNE
NNN
ENE
EEN
EEE

stationary structures for the orientations of the surface hydroxide groups in the order of alpha, beta, beta (clockwise) as a function of level of theory

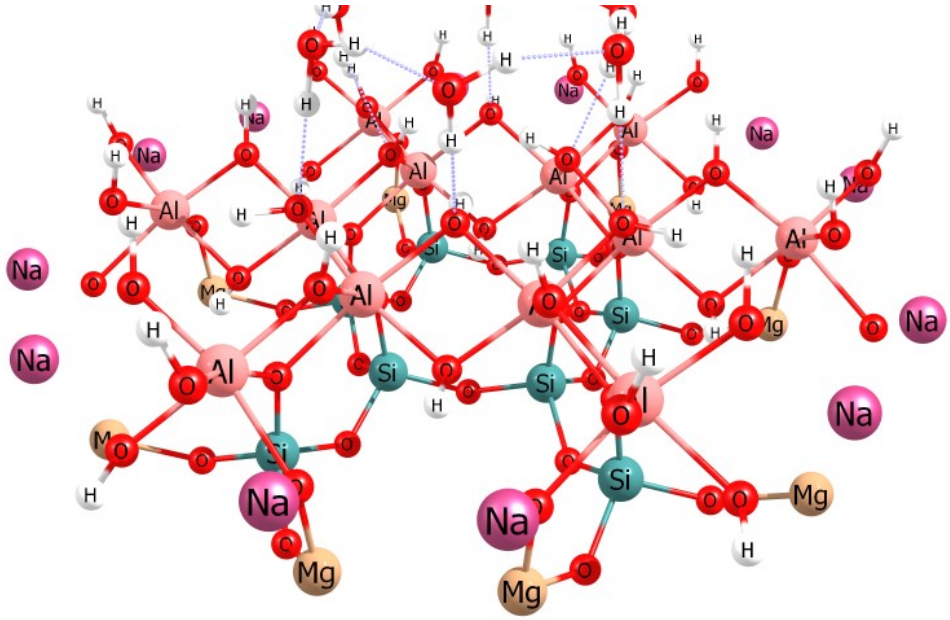
HF/def2TZVP	PW91/def2TZVP	B3LYP/def2TZVP
NEE	NNE	NEE
NNE	NEN	NNE
NEN	ENN	NEN
	NEE	ENN

explicit water nano-droplet $(H_2O)_6$) interaction with the surface in aqueous media

initial 64 structures for all possible combinations of proximal surface hydroxide groups and H-bond donor (D) acceptor (A) positions of the 6-membered water-ring cluster

AAAAAA	ADAAAA	DAAAAA	DDAAAA
AAAAAD	ADAAAD	DAAAAD	DDAAAD
AAAADA	ADAADA	DAAADA	DDAADA
AAAADD	ADAADD	DAAADD	DDAADD
AAADAA	ADADAA	DAADAA	DDADAA
AAADAD	ADADAD	DAADAD	DDADAD
AAADDA	ADADDA	DAADDA	DDADDA
AAADDD	ADADDD	DAADDD	DDADDD
AADAAA	ADDAAA	DADAAA	DDDAAA
AADAAD	ADDAAD	DADAAD	DDDAAD
AADADA	ADDADA	DADADA	DDDADA
AADADD	ADDADD	DADADD	DDDADD
AADDAA	ADDDAA	DADDAA	DDDDAA
AADDAD	ADDDAD	DADDAD	DDDDAD
AADDDA	ADDDDA	DADDDA	DDDDDA
AADDDD	ADDDDD	DADDDD	DDDDDD

stationary structures for the position of the water nano-droplet at the Al-surface as a function of level of theory

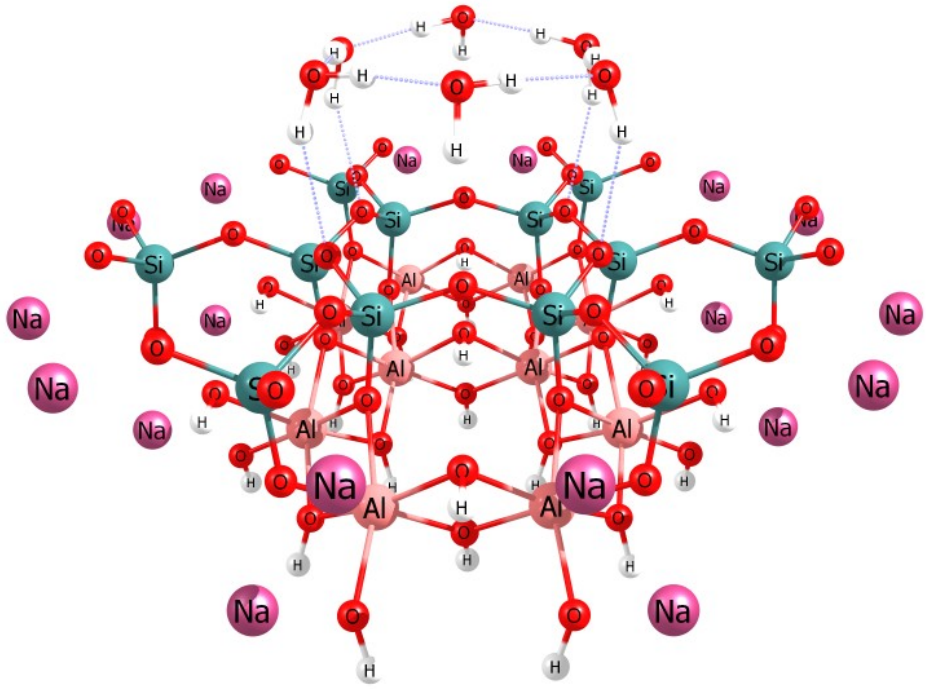


B3LYP/def2TZVP	B3LYP+D/def2TZVP+PCM
AAA	AAA
AAD	
ADA	ADA
ADD	ADD
DAA	DAA
DAD	DAD
DDA	DDA

Tetrahedral Layer - [6Si-6(*b*-O^{2-})] honeycomb

explicit water nano-droplet $(H_2O)_6$ interaction with the surface in aqueous media

stationary structures for the position of the water nano-droplet at the Al-surface as a function of level of theory



B3LYP/def2TZVP +PCM +Dispersion&PCM

Download here the entire database (340 kb) of structures in XYZ format