Supporting Information for:
“Toward Accurate Adsorption Energetics on Clay Surfaces”

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We report here a detailed description of the computational setups for the calculations performed in this work. In particular, Section 1 is about DMC, Section 2 about LRDMC, Section 3 about the finite-size effects in QMC, and Section 4 about DFT.

Moreover, in Table S1 we report the adsorption energy obtained, for the reference PBE-D3 optimized structures (used for QMC), using several DFT functionals, including LDA, GGA, meta-GGA and hybrid type. GGA functionals used include the Perdew-Burke-Ernzerhof (PBE)1,2, RPBE3 and Becke-Lee-Yang-Parr (BLYP)4,5. SCAN is a meta-GGA functional6. Hybrid functionals considered are the PBE07, HSE068 and B3LYP9–12 functionals. Van der Waals corrections were accounted in several different schemes. The first is the D2 and D3 corrections of Grimme13,14, and in parenthesis BJ indicates a Becke and Johnson damping (instead of the zero-damping)15 and ATM indicates the use of a nonadditive three-body dispersion term of Axilrod-Teller-Muto type. The second is the corrections of Tkatchenko and Scheffler (+vdW(TS))16, also with the self-consistent screening (+vdW(TS-scs))17. Results for the van der Waals functionals vdW-DF, vdW-DF2, optPBE-vdW and optB86b-vdW are also reported18–21.

Finally, we provide the structures, in .cif file format, used for the DMC and LRDMC calculations. As described in the main paper, these structures have been obtained through a DFT-base relaxation, using the PBE-D3 functional.
Table S1: Adsorption Energy [meV] of water (W) and methanol (M) molecules on the hydroxyl-terminated (AlOH) and silicate-terminated (SiO₂) faces of kaolinite. All evaluations have been performed on the reference structures obtained from PBE-D3 based relaxation, and used also for the DMC calculations. Functionals are defined in the text.

|         | W@AlOH | M@AlOH | W@SiO₂ | M@SiO₂ |
|---------|--------|--------|--------|--------|
| LDA     | -1102  | -1138  | -295   | -315   |
| PBE     | -607   | -614   | -85    | -93    |
| PBE-D2  | -822   | -879   | -262   | -331   |
| PBE-D3  | -767   | -828   | -248   | -314   |
| PBE-D3(ATM) | -757   | -814   | -241   | -300   |
| PBE-D3(BJ) | -766   | -827   | -245   | -313   |
| PBE-D3(BJ,ATM) | -757   | -812   | -237   | -299   |
| PBE+vdW(TS) | -769   | -841   | -271   | -356   |
| RPBE    | -360   | -354   | 25     | 21     |
| RPBE-D3 | -697   | -749   | -261   | -328   |
| RPBE-D3(ATM) | -688   | -735   | -253   | -314   |
| RPBE-D3(BJ) | -721   | -783   | -266   | -343   |
| RPBE-D3(BJ,ATM) | -712   | -768   | -258   | -330   |
| BLYP    | -470   | -463   | 10     | 24     |
| BLYP-D2 | -815   | -888   | -273   | -357   |
| BLYP-D3 | -764   | -830   | -293   | -368   |
| BLYP-D3(ATM) | -755   | -816   | -285   | -354   |
| BLYP-D3(BJ) | -756   | -832   | -276   | -359   |
| BLYP-D3(BJ,ATM) | -747   | -817   | -268   | -345   |
| vdW-DF  | -530   | -597   | -183   | -297   |
| vdW-DF2 | -616   | -658   | -210   | -292   |
| optPBE-vdW | -689   | -767   | -248   | -369   |
| optB86b-vdW | -751   | -835   | -236   | -350   |
| SCAN    | -707   | -728   | -160   | -181   |
| SCAN-D3 | -777   | -838   | -226   | -284   |
| SCAN-D3(ATM) | -768   | -823   | -218   | -270   |
| SCAN-D3(BJ) | -805   | -866   | -258   | -322   |
| SCAN-D3(BJ,ATM) | -796   | -852   | -250   | -308   |
| PBE0    | -599   | -615   | -75    | -86    |
| PBE0-D2 | -771   | -827   | -217   | -277   |
| PBE0-D3 | -768   | -840   | -241   | -311   |
| PBE0-D3(ATM) | -759   | -825   | -233   | -297   |
| PBE0-D3(BJ) | -750   | -823   | -233   | -307   |
| PBE0-D3(BJ,ATM) | -741   | -808   | -225   | -293   |
| PBE0+vdW(TS-scs) | -784   | -869   | -255   | -333   |
| HSE06   | -596   | -608   | -70    | -73    |
| HSE06-D3 | -716   | -776   | -203   | -255   |
| HSE06-D3(ATM) | -707   | -762   | -195   | -242   |
| HSE06-D3(BJ) | -736   | -809   | -221   | -294   |
| HSE06-D3(BJ,ATM) | -727   | -794   | -213   | -280   |
| HSE06+vdW(TS) | -758   | -835   | -255   | -335   |
| B3LYP   | -524   | -528   | -24    | -19    |
| B3LYP-D2 | -826   | -900   | -272   | -352   |
| B3LYP-D3 | -776   | -849   | -273   | -345   |
| B3LYP-D3(ATM) | -767   | -834   | -265   | -331   |
| B3LYP-D3(BJ) | -764   | -840   | -265   | -343   |
| B3LYP-D3(BJ,ATM) | -755   | -826   | -257   | -330   |
| B3LYP+vdW(TS-scs) | -799   | -893   | -278   | -343   |
1 DMC setup

DMC calculations were performed using the CASINO code. A Slater-Jastrow wave-function ansatz is used as a guiding function for the importance sampling DMC calculations. Trail and Needs PPs are used for all atoms in the system. The Slater determinant is obtained from DFT-LDA plane-wave calculations using PWSCF with a 600 Ry energy cutoff. The resulting molecular orbitals were expanded in terms of B-splines. The Jastrow factor contains electron-electron, electron-nucleus, and electron-electron-nucleus terms, which have been optimized, within a variational Monte Carlo (VMC) scheme, via minimization of the VMC variance. The DMC calculations were performed within the fixed-node approximation and non-local terms in the PPs were handled by using the locality approximation. Umrigar et al.’s scheme for the branching-drift-diffusion process is adopted, with a time-step $\tau$ of 0.005 a.u. The adsorption energies were evaluated using the complex-minus-far method, see Eq. 2 in main paper.

For each configuration considered, we used a target population of 204,800 walkers across 20,480 physical nodes (1280 computational nodes on Titan supercomputer) and we simulated more than 15,000 DMC time steps: the first 1,000 for equilibration; the remaining averaged using the “blocking” method with a bin of 512. This setup guarantees evaluations of the absolute energy of each configuration with an associated stochastic error of $\sim 13$ meV, giving an error of $\sim 20$ meV on the adsorption energies.

2 LRDMC setup

The LRDMC results reported have been obtained with the TurboRVB package developed by Sorella and coworkers. The setup for the LRDMC calculations slightly differs from that of the DMC calculations as a consequence of the different implementations of the algorithms in TurboRVB and CASINO. The main differences are in the variational wave function: orbitals in TurboRVB are expressed in terms of localized basis functions (of Gaussian, Slater and other types), and the Jastrow factor is parametrized differently. The wave function ansatz implemented in TurboRVB is the Jastrow Antisymmetrized Geminal Power, which includes the Slater-Jastrow ansatz as a special branching-drift-diffusion algorithm, so that now much larger $\tau$ can be used. However, the calculations presented here were performed before the aforementioned developments.
Moreover, the parameters of the variational wave function (to be used as the guiding function for the LRDMC calculation) are optimized in order to minimize the variational energy. For a more detailed description of the wave function implemented in TurboRVB see Ref. 48.

In this work we have used a Slater-Jastrow wave function. Core electrons of C, O, Al and Si atoms have been described via scalar-relativistic energy-consistent Hartree-Fock PPs of Burkatzki et al. Consistent with the choice of the PP, the basis set has been obtained starting from the Burkatzki et al. VTZ basis set. For use in the TurboRVB package, we have uncontracted the basis set and removed the almost redundant exponents and those too small or too large in value (keeping these would imply a much slower and inefficient optimization of the wave-function parameters, with an almost negligible energy gain), obtaining (7s,2p) for H atoms, (11s,11p,2d) for C, (10s,11p,2d) for O, (11s,11p,2d,1f) for Al and Si. The coefficients of the molecular orbitals have then been optimized by performing a DFT-LDA calculation, using the DFT code included in the TurboRVB package. The Jastrow factor used here consists of both homogeneous and non-homogeneous terms that account for the electron-electron, electron-nucleus and electron-electron-nucleus interactions. The non-homogeneous terms are expressed in terms of atomic orbitals, which are expanded in terms of (2s,2p) basis for H atoms, (3s,2p,1d) for C and O atoms, (3s,2p,2d) for Al and Si atoms. The exponents of the Jastrow atomic orbitals have been fixed to the values obtained from the optimization in a smaller model system. All the other parameters of the Jastrow factor have been optimized for each specific configuration. In the LRDMC we used a mesh $a$ of 0.4 a.u.

Since we are evaluating the adsorption energy in weakly interacting systems, we expect that the above setup leads to unbiased results, in particular with respect to the choice of the basis set and the LRDMC mesh $a$. See e.g. Ref. 40 for results on the water dimer. However, here we have also checked directly whether the above setup leads to unbiased results for the kaolinite plus water/methanol system, by performing tests on model systems (i.e., a molecule bound to a cluster representing kaolinite). We observed that the adsorption energies obtained with $a = 0.4$ a.u. are the same, within error bars, as those obtained with $a = 0.1$ and 0.2 a.u. Moreover, by performing additional calculations with different basis sets, we ascertained that with the chosen setup we have no basis-set bias at the LRDMC level.

TurboRVB allows one to perform calculations with open conditions or with 3D periodic boundary conditions. Unfortunately, 2D periodic boundary conditions are not yet implemented in the code. This makes the use of the complex-minus-far evaluation of the adsorption energy problematic. On the other hand, LRDMC is size consistent for any mesh $a$. Thus, we have chosen the complex-minus-fragments approach here, see Eq. 1 in the main paper. As described in Section 3, we have used the KZK method to evaluate the finite-size effects (Table S2 and LRDMC evaluations have been corrected accordingly. The effect of the dipole interactions perpendicular to the slab have been corrected on the basis of DFT-based estimates of the effect. Namely, in the reported LRDMC calculations there is a vacuum between the slabs of $\sim 15$ Å, for which DFT predicts that the adsorption energy without dipole correction would result in a 36 meV underestimation for water on the hydroxyl-terminated face, and a 38 meV underestimation for methanol.

3 Finite-size effects in QMC

FSEs in our QMC evaluations have been evaluated using the KZK method. This method is pretty simple and computationally cheap: we have to perform two DFT calculations for each complex considered, the first with the LDA functional and the second with the KZK functional (which mimics the FSE in many-body electronic structure calculations). The difference between the two evaluations provides an estimate of the FSE in QMC. KZK corrections
have been calculated using the implementation in PWSCF\textsuperscript{27} due to E. Sola, as reported in Ref. \textsuperscript{52}, with the setup previously described to generate the Slater determinant of the guiding function. In this way we have seen that FSEs are relatively large in the absolute energy of the complexes (KZK predicts an underestimation of $\sim 1.3$ eV on the absolute energy), but there is a huge error cancellation in the evaluation of the adsorption energy: according to KZK the QMC evaluation with the complex-minus-far method leads to an underestimate $|E_{\text{ads}}^{M@X}|$ of 12 - 17 meV, depending on the surface and on the molecule considered (Table S2). On the other hand, if the complex-minus-fragments method is used, error cancellation is slightly worse and the correction has the opposite sign: $|E_{\text{ads}}^{H_2O@X}|$ is overestimated by $\sim 35$ meV ($X$ being either the hydroxyl-terminated face, AlOH, or the silicate-terminated face, SiO$_2$), whereas $|E_{\text{ads}}^{MeOH@X}|$ is overestimated by $\sim 75$ meV. Thus, the complex-minus-far method is to be preferred in terms of FSEs.

Table S2: The following table summarizes the KZK\textsuperscript{43} evaluations of the FSE on the adsorption energy of the different systems considered, either by using the complex-minus-fragments evaluation, Eq. 1 in the main paper, or the complex-minus-far, Eq. 2 in the main paper. Here, a positive value implies that the absolute value of $E_{\text{ads}}^{M@X}$ is overestimated if the bare QMC value is taken; a negative value indicates an underestimation.

|               | complex-minus-fragments | far |
|---------------|-------------------------|-----|
|               | Eq. 1 | Eq. 2 |
| $H_2O@AlOH$   | +35   | -16  |
| $MeOH@AlOH$   | +73   | -17  |
| $H_2O@SiO_2$  | +38   | -12  |
| $MeOH@SiO_2$  | +76   | -14  |

4 DFT setup

DFT calculations were performed using the plane-wave code VASP 5.4.\textsuperscript{53-56} Calculations using the van der Waals density functionals were carried out self-consistently using the approach of Román-Pérez and Soler\textsuperscript{57} as implemented in VASP by Klimes \textit{et al.}\textsuperscript{21} Electron-core interactions were described using the projector-augmented wave\textsuperscript{58,59} (PAW) potentials supplied with VASP. PBE PAW potentials for all functionals were used, with the exception of LDA where LDA PAW was used. It has been shown on a range of systems for the vdW functionals that this approximation with the PAW functionals does not introduce significant errors in the energies and structures.\textsuperscript{21,60}

Adsorption energies were evaluated using the complex-minus-fragments method, see Eq. 1 in the main paper, because we have close-shell systems, where DFT is exactly size-consistent, and the system is large enough to have negligible size-effects. $E_M$ was calculated at the $\Gamma$-point by isolating a single molecule in a $20 \times 20 \times 20$ Å box. For the calculation of $E_{\text{slab}}$ and $E_{\text{slab}+M@X}$ we used three dimensional periodicity with a vacuum region between slabs of ca. 15 Å, and the dipole interaction across the slab was corrected with the scheme of Neugebauer and Scheffler,\textsuperscript{61,62} in order to mimic a 2D system, and $\Gamma$-point sampling of reciprocal space. For all adsorption calculations, a plane-wave energy cut-off of 500 eV was used. During structure optimizations all atoms were fully relaxed until the forces were reduced below $10^{-3}$ eV/Å.
### Water Molecule

```
data_water
  _symmetry_Int_Tables_number 1
  _cell_length_a  20.000000
  _cell_length_b  20.000000
  _cell_length_c  20.000000
  _cell_angle_alpha 90.000000
  _cell_angle_beta  90.000000
  _cell_angle_gamma 90.000000

  loop_
    _symmetry_equiv_pos_site_id 1
    _symmetry_equiv_pos_as_xyz x, y, z

  loop_
    _atom_site_label O1
    _atom_site_type_symbol O
    _atom_site_fract_x  0.16139
    _atom_site_fract_y  0.22133
    _atom_site_fract_z  0.33630
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H1
    _atom_site_type_symbol H
    _atom_site_fract_x  0.14296
    _atom_site_fract_y  0.20583
    _atom_site_fract_z  0.37851
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H2
    _atom_site_type_symbol H
    _atom_site_fract_x  0.14227
    _atom_site_fract_y  0.19157
    _atom_site_fract_z  0.30298
    _atom_site_occupancy  1.0000
```

### Methanol Molecule

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data_methanol
  _symmetry_Int_Tables_number 1
  _cell_length_a  20.000000
  _cell_length_b  20.000000
  _cell_length_c  20.000000
  _cell_angle_alpha 90.000000
  _cell_angle_beta  90.000000
  _cell_angle_gamma 90.000000

  loop_
    _symmetry_equiv_pos_site_id 1
    _symmetry_equiv_pos_as_xyz x, y, z

  loop_
    _atom_site_label O1
    _atom_site_type_symbol O
    _atom_site_fract_x  0.15721
    _atom_site_fract_y  0.22210
    _atom_site_fract_z  0.33789
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H1
    _atom_site_type_symbol H
    _atom_site_fract_x  0.14581
    _atom_site_fract_y  0.19214
    _atom_site_fract_z  0.30141
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H2
    _atom_site_type_symbol H
    _atom_site_fract_x  0.06137
    _atom_site_fract_y  0.21459
    _atom_site_fract_z  0.38181
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H3
    _atom_site_type_symbol H
    _atom_site_fract_x  0.12872
    _atom_site_fract_y  0.24160
    _atom_site_fract_z  0.43372
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label H4
    _atom_site_type_symbol H
    _atom_site_fract_x  0.12187
    _atom_site_fract_y  0.15537
    _atom_site_fract_z  0.41185
    _atom_site_occupancy  1.0000

  loop_
    _atom_site_label C1
    _atom_site_type_symbol C
    _atom_site_fract_x  0.11476
    _atom_site_fract_y  0.20696
    _atom_site_fract_z  0.39355
    _atom_site_occupancy  1.0000
```

# Kaolinite slab

data_KAOslab

| symmetry_Int_Tables_number | 1 |
|---------------------------|---|
| _cell_length_a            | 10.384527 |
| _cell_length_b            | 9.011475  |
| _cell_length_c            | 22.250826 |
| _cell_angle_alpha         | 90.000000 |
| _cell_angle_beta          | 90.000000 |
| _cell_angle_gamma         | 90.000000 |

| symmetry_equiv_pos_site_id | x, y, z |
|---------------------------|--------|
| 1                         | x, y, z |

| atom_site_label    | atom_site_type_symbol | atom_site_fract_x | atom_site_fract_y | atom_site_fract_z | atom_site_occupancy |
|--------------------|-----------------------|-------------------|-------------------|-------------------|---------------------|
| Al1                | Al                    | 0.14470           | 0.49573           | 0.15530           | 1.0000              |
| Al2                | Al                    | 0.14194           | 0.83066           | 0.15527           | 1.0000              |
| Al3                | Al                    | 0.39470           | 0.99573           | 0.15530           | 1.0000              |
| Al4                | Al                    | 0.39194           | 0.33066           | 0.15527           | 1.0000              |
| Al5                | Al                    | 0.64470           | 0.49573           | 0.15530           | 1.0000              |
| Al6                | Al                    | 0.64194           | 0.83066           | 0.15527           | 1.0000              |
| Al7                | Al                    | 0.89470           | 0.99573           | 0.15530           | 1.0000              |
| Al8                | Al                    | 0.89194           | 0.33066           | 0.15527           | 1.0000              |
| Si1                | Si                    | 0.06153           | 0.34406           | 0.03339           | 1.0000              |
| Si2                | Si                    | 0.06981           | 0.67178           | 0.03336           | 1.0000              |
| Si3                | Si                    | 0.31153           | 0.84406           | 0.03339           | 1.0000              |
| Si4                | Si                    | 0.31981           | 0.17178           | 0.03336           | 1.0000              |
| Si5                | Si                    | 0.56153           | 0.34406           | 0.03339           | 1.0000              |
| Si6                | Si                    | 0.56981           | 0.67178           | 0.03336           | 1.0000              |
| Si7                | Si                    | 0.81153           | 0.84406           | 0.03339           | 1.0000              |
| Si8                | Si                    | 0.81981           | 0.17178           | 0.03336           | 1.0000              |
| O1                 | O                     | 0.04590           | 0.35865           | 0.10686           | 1.0000              |
| O2                 | O                     | 0.08879           | 0.66353           | 0.10683           | 1.0000              |
| O3                 | O                     | 0.09137           | 0.50668           | 0.00490           | 1.0000              |
| O4                 | O                     | 0.17404           | 0.22476           | 0.01699           | 1.0000              |
| O5                 | O                     | 0.17675           | 0.78321           | 0.00480           | 1.0000              |
| O6                 | O                     | 0.29590           | 0.85865           | 0.10686           | 1.0000              |
| O7                 | O                     | 0.33879           | 0.16353           | 0.10683           | 1.0000              |
| O8                 | O                     | 0.34137           | 0.00668           | 0.00490           | 1.0000              |
| O9                 | O                     | 0.42404           | 0.72476           | 0.01699           | 1.0000              |
| O10                | O                     | 0.42675           | 0.28321           | 0.00480           | 1.0000              |
| O11                | O                     | 0.04652           | 0.96964           | 0.10954           | 1.0000              |
| O12                | O                     | 0.45538           | 0.16288           | 0.19990           | 1.0000              |
| O13                | O                     | 0.98712           | 0.47498           | 0.19984           | 1.0000              |
| O14                | O                     | 0.98506           | 0.84663           | 0.20102           | 1.0000              |
| O15                | O                     | 0.29652           | 0.96964           | 0.10954           | 1.0000              |
| O16                | O                     | 0.20538           | 0.66288           | 0.19990           | 1.0000              |
| O17                | O                     | 0.23712           | 0.97498           | 0.19984           | 1.0000              |
| O18                | O                     | 0.23506           | 0.34663           | 0.20102           | 1.0000              |
| O19                | O                     | 0.54590           | 0.35865           | 0.10686           | 1.0000              |
| O20                | O                     | 0.58879           | 0.66353           | 0.10683           | 1.0000              |
| O21                | O                     | 0.59137           | 0.50668           | 0.00490           | 1.0000              |
| O22                | O                     | 0.67404           | 0.22476           | 0.01699           | 1.0000              |
| O23                | O                     | 0.67675           | 0.78321           | 0.00480           | 1.0000              |
| O24                | O                     | 0.79590           | 0.85865           | 0.10686           | 1.0000              |
| O25                | O                     | 0.83879           | 0.16353           | 0.10683           | 1.0000              |
| O26                | O                     | 0.84137           | 0.00668           | 0.00490           | 1.0000              |
| O27                | O                     | 0.92404           | 0.72476           | 0.01699           | 1.0000              |
| O28                | O                     | 0.92675           | 0.28321           | 0.00480           | 1.0000              |
| O29                | O                     | 0.54652           | 0.96964           | 0.10954           | 1.0000              |
| O30                | O                     | 0.95538           | 0.16288           | 0.19990           | 1.0000              |
| O31                | O                     | 0.48712           | 0.47498           | 0.19984           | 1.0000              |
| O32                | O                     | 0.48506           | 0.84663           | 0.20102           | 1.0000              |
| O33                | O                     | 0.79652           | 0.46964           | 0.10954           | 1.0000              |
| O34                | O                     | 0.70538           | 0.66288           | 0.19990           | 1.0000              |
| O35                | O                     | 0.73712           | 0.97498           | 0.19984           | 1.0000              |
# Kaolinite slab + 1 water at AlOH

```
data_ALOHwith1w

_symmetry_Int_Tables_number 1
_cell_length_a 10.384527
_cell_length_b 9.011475
_cell_length_c 22.250826
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_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000
loop_
symmetry_equiv_pos_site_id
symmetry_equiv_pos_as_xyz
  1 x,y,z
loop_
atom_site_label
atom_site_type_symbol
atom_site_fract_x
atom_site_fract_y
atom_site_fract_z
atom_site_occupancy
Al1 Al 0.14572 0.49631 0.15560 1.0000
Al2 Al 0.13591 0.83014 0.15686 1.0000
Al3 Al 0.38792 0.99569 0.15503 1.0000
Al4 Al 0.39838 0.32793 0.15529 1.0000
Al5 Al 0.64615 0.49650 0.15677 1.0000
Al6 Al 0.63612 0.83040 0.15517 1.0000
Al7 Al 0.88697 0.99664 0.15555 1.0000
Al8 Al 0.89416 0.32876 0.15696 1.0000
Si1 Si 0.06027 0.34270 0.03414 1.0000
Si2 Si 0.06643 0.67123 0.03420 1.0000
Si3 Si 0.30754 0.84349 0.03416 1.0000
Si4 Si 0.31668 0.17140 0.03359 1.0000
Si5 Si 0.56059 0.34305 0.03344 1.0000
Si6 Si 0.56681 0.67089 0.03381 1.0000
Si7 Si 0.80777 0.84363 0.03385 1.0000
Si8 Si 0.81709 0.17168 0.03404 1.0000
O1 O 0.04871 0.35378 0.10797 1.0000
O2 O 0.08554 0.66233 0.10762 1.0000
O3 O 0.08838 0.50611 0.00604 1.0000
O4 O 0.17215 0.22484 0.01549 1.0000
O5 O 0.17297 0.78273 0.00531 1.0000
O6 O 0.28947 0.85954 0.10744 1.0000
O7 O 0.33241 0.16435 0.10721 1.0000
O8 O 0.33885 0.00574 0.00560 1.0000
O9 O 0.42033 0.72372 0.01851 1.0000
O10 O 0.42509 0.28198 0.00579 1.0000
O11 O 0.04181 0.97011 0.11110 1.0000
O12 O 0.45249 0.15700 0.20115 1.0000
O13 O 0.99614 0.46321 0.20134 1.0000
O14 O 0.97613 0.84603 0.20082 1.0000
O15 O 0.29793 0.46861 0.11091 1.0000
O16 O 0.20064 0.66425 0.20058 1.0000
O17 O 0.22945 0.98055 0.20185 1.0000
O18 O 0.24370 0.34713 0.20337 1.0000
O19 O 0.31793 0.17168 0.29778 1.0000
O20 O 0.54903 0.35564 0.10711 1.0000
O21 O 0.58739 0.66159 0.10711 1.0000
O22 O 0.58837 0.50623 0.00503 1.0000
O23 O 0.67242 0.22441 0.01561 1.0000
O24 O 0.67300 0.78324 0.00500 1.0000
O25 O 0.79036 0.85898 0.10722 1.0000
O26 O 0.83312 0.16477 0.10758 1.0000
O27 O 0.83922 0.00574 0.00580 1.0000
O28 O 0.92044 0.72405 0.01810 1.0000
O29 O 0.92484 0.28278 0.00613 1.0000
O30 O 0.54084 0.96827 0.10913 1.0000
O31 O 0.94273 0.15777 0.20305 1.0000
O32 O 0.49242 0.46912 0.20034 1.0000
O33 O 0.47755 0.84342 0.19956 1.0000
O34 O 0.79856 0.47105 0.20305 1.0000
O35 O 0.70418 0.66798 0.20153 1.0000
```
```
# Kaolinite slab + water at SiO2

data_SiO2+W

_symmetry_Int_Tables_number 1
_cell_length_a 10.384527
_cell_length_b 9.011475
_cell_length_c 22.250826
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 90.000000

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1 Al 0.34494 0.47202 0.59779 1.0000
Al2 Al 0.34550 0.80745 0.59805 1.0000
Al3 Al 0.59946 0.97205 0.59703 1.0000
Al4 Al 0.59381 0.30859 0.59651 1.0000
Al5 Al 0.84692 0.47407 0.59645 1.0000
Al6 Al 0.84800 0.80630 0.59697 1.0000
Al7 Al 0.09764 0.97474 0.59829 1.0000
Al8 Al 0.09436 0.30672 0.59685 1.0000
Si1 Si 0.26537 0.31908 0.47519 1.0000
Si2 Si 0.27234 0.64832 0.47582 1.0000
Si3 Si 0.51447 0.81984 0.47540 1.0000
Si4 Si 0.52354 0.14750 0.47476 1.0000
Si5 Si 0.76535 0.32042 0.47501 1.0000
Si6 Si 0.77299 0.64823 0.47498 1.0000
Si7 Si 0.01538 0.81978 0.47575 1.0000
Si8 Si 0.02332 0.14733 0.47520 1.0000
O1 O 0.25025 0.33147 0.54851 1.0000
O2 O 0.29007 0.64073 0.54925 1.0000
O3 O 0.29484 0.48295 0.44711 1.0000
O4 O 0.37890 0.20231 0.45758 1.0000
O5 O 0.37943 0.75908 0.44717 1.0000
O6 O 0.49910 0.44771 0.54896 1.0000
O7 O 0.49910 0.23318 0.45758 1.0000
O8 O 0.49910 0.14224 0.45758 1.0000
O9 O 0.00181 0.83324 0.54934 1.0000
O10 O 0.04070 0.13964 0.54872 1.0000
O11 O 0.04530 0.98220 0.44716 1.0000
O12 O 0.04704 0.32191 0.64224 1.0000
O13 O 0.51495 0.47869 0.34562 1.0000
O14 O 0.74774 0.33569 0.54828 1.0000
O15 O 0.79290 0.64013 0.54852 1.0000
O16 O 0.79543 0.48300 0.44667 1.0000
O17 O 0.87738 0.20049 0.45888 1.0000
O18 O 0.87996 0.76057 0.44725 1.0000
O19 O 0.00181 0.83324 0.54934 1.0000
O20 O 0.04070 0.13964 0.54872 1.0000
O21 O 0.04530 0.98220 0.44716 1.0000
O22 O 0.04704 0.32191 0.64224 1.0000
O23 O 0.51495 0.47869 0.34562 1.0000
O24 O 0.74774 0.33569 0.54828 1.0000
O25 O 0.79290 0.64013 0.54852 1.0000
O26 O 0.79543 0.48300 0.44667 1.0000
O27 O 0.87738 0.20049 0.45888 1.0000
O28 O 0.87996 0.76057 0.44725 1.0000
O29 O 0.00181 0.83324 0.54934 1.0000
O30 O 0.04070 0.13964 0.54872 1.0000
O31 O 0.04530 0.98220 0.44716 1.0000
O32 O 0.04704 0.32191 0.64224 1.0000
O33 O 0.51495 0.47869 0.34562 1.0000
O34 O 0.74774 0.33569 0.54828 1.0000
O35 O 0.79290 0.64013 0.54852 1.0000
O36 O 0.94427 0.94201 0.64450 1.0000
O37 O 0.93427 0.32447 0.64144 1.0000
H1 H 0.43587 0.49030 0.36860 1.0000
H2 H 0.56271 0.40337 0.36764 1.0000
H3 H 0.29371 0.03197 0.53517 1.0000
H4 H 0.64106 0.14224 0.68505 1.0000
H5 H 0.13288 0.53615 0.64680 1.0000
H6 H 0.64211 0.72970 0.64444 1.0000
H7 H 0.53957 0.53111 0.53199 1.0000
H8 H 0.40122 0.63497 0.68605 1.0000
H9 H 0.43696 0.95803 0.68512 1.0000
H10 H 0.38879 0.22929 0.64480 1.0000
H11 H 0.79145 0.02621 0.52857 1.0000
H12 H 0.15692 0.14701 0.68527 1.0000
H13 H 0.68856 0.45203 0.68458 1.0000
H14 H 0.14078 0.75647 0.66274 1.0000
H15 H 0.03868 0.52300 0.52633 1.0000
H16 H 0.89666 0.64275 0.68496 1.0000
H17 H 0.89743 0.01709 0.66646 1.0000
H18 H 0.87914 0.23718 0.64143 1.0000
# Kaolinite slab + 1 methanol at AlOH

data_ALOH+M

| symmetry_Int_Tables_number | 1 |
|---------------------------|---|
| cell_length_a             | 10.384527 |
| cell_length_b             | 9.011475 |
| cell_length_c             | 22.250826 |
| cell_angle_alpha          | 90.000000 |
| cell_angle_beta           | 90.000000 |
| cell_angle_gamma          | 90.000000 |

| symmetry_equiv_pos_site_id | x, y, z |
|---------------------------|--------|
| 1                         | x, y, z |

| atom_site_label | atom_site_type_symbol | atom_site_fract_x | atom_site_fract_y | atom_site_fract_z | atom_site_occupancy |
|----------------|----------------------|------------------|------------------|------------------|---------------------|
| Al1            | Al                   | 0.14576          | 0.49695          | 0.15682          | 1.0000              |
| Al2            | Al                   | 0.13620          | 0.83081          | 0.15827          | 1.0000              |
| Al3            | Al                   | 0.38826          | 0.99635          | 0.15634          | 1.0000              |
| Al4            | Al                   | 0.39861          | 0.32858          | 0.15643          | 1.0000              |
| Al5            | Al                   | 0.64618          | 0.49724          | 0.15812          | 1.0000              |
| Al6            | Al                   | 0.63646          | 0.83107          | 0.15645          | 1.0000              |
| Al7            | Al                   | 0.88729          | 0.99738          | 0.15689          | 1.0000              |
| Al8            | Al                   | 0.89426          | 0.32946          | 0.15834          | 1.0000              |
| Si1            | Si                   | 0.06062          | 0.34334          | 0.03547          | 1.0000              |
| Si2            | Si                   | 0.06664          | 0.67194          | 0.03554          | 1.0000              |
| Si3            | Si                   | 0.30782          | 0.84413          | 0.03548          | 1.0000              |
| Si4            | Si                   | 0.31704          | 0.17200          | 0.03483          | 1.0000              |
| Si5            | Si                   | 0.56096          | 0.34371          | 0.03471          | 1.0000              |
| Si6            | Si                   | 0.56711          | 0.67158          | 0.03511          | 1.0000              |
| Si7            | Si                   | 0.80806          | 0.84432          | 0.03514          | 1.0000              |
| Si8            | Si                   | 0.81747          | 0.17235          | 0.03538          | 1.0000              |
| O1             | O                   | 0.04890          | 0.35433          | 0.10929          | 1.0000              |
| O2             | O                   | 0.08555          | 0.66311          | 0.10898          | 1.0000              |
| O3             | O                   | 0.08872          | 0.50681          | 0.00742          | 1.0000              |
| O4             | O                   | 0.17255          | 0.22559          | 0.01678          | 1.0000              |
| O5             | O                   | 0.17323          | 0.78338          | 0.00665          | 1.0000              |
| O6             | O                   | 0.28976          | 0.86018          | 0.10877          | 1.0000              |
| O7             | O                   | 0.33273          | 0.16493          | 0.01678          | 1.0000              |
| O8             | O                   | 0.35020          | 0.98901          | 0.20323          | 1.0000              |
| O9             | O                   | 0.42057          | 0.72427          | 0.01984          | 1.0000              |
| O10            | O                   | 0.42551          | 0.28255          | 0.00704          | 1.0000              |
| O11            | O                   | 0.04222          | 0.97089          | 0.11252          | 1.0000              |
| O12            | O                   | 0.94257          | 0.15853          | 0.20438          | 1.0000              |
| O13            | O                   | 0.99667          | 0.46313          | 0.20290          | 1.0000              |
| O14            | O                   | 0.97623          | 0.84676          | 0.20219          | 1.0000              |
| O15            | O                   | 0.29802          | 0.49392          | 0.11210          | 1.0000              |
| O16            | O                   | 0.20059          | 0.66472          | 0.20193          | 1.0000              |
| O17            | O                   | 0.23000          | 0.98901          | 0.20323          | 1.0000              |
| O18            | O                   | 0.24377          | 0.34761          | 0.20436          | 1.0000              |
| O19            | O                   | 0.32008          | 0.50831          | 0.29792          | 1.0000              |
| O20            | O                   | 0.54933          | 0.35624          | 0.10837          | 1.0000              |
| O21            | O                   | 0.58776          | 0.66230          | 0.10841          | 1.0000              |
| O22            | O                   | 0.58878          | 0.50692          | 0.00633          | 1.0000              |
| O23            | O                   | 0.67284          | 0.22510          | 0.01692          | 1.0000              |
| O24            | O                   | 0.67326          | 0.78397          | 0.00629          | 1.0000              |
| O25            | O                   | 0.79074          | 0.85963          | 0.10852          | 1.0000              |
| O26            | O                   | 0.83342          | 0.16566          | 0.10892          | 1.0000              |
| O27            | O                   | 0.83959          | 0.00693          | 0.00712          | 1.0000              |
| O28            | O                   | 0.92066          | 0.72467          | 0.01936          | 1.0000              |
| O29            | O                   | 0.92521          | 0.28342          | 0.00744          | 1.0000              |
| O30            | O                   | 0.54113          | 0.96887          | 0.11040          | 1.0000              |
| O31            | O                   | 0.45282          | 0.15774          | 0.20242          | 1.0000              |
| O32            | O                   | 0.49249          | 0.46964          | 0.20156          | 1.0000              |
| O33            | O                   | 0.47790          | 0.84405          | 0.20088          | 1.0000              |
| O34            | O                   | 0.79878          | 0.47179          | 0.12354          | 1.0000              |
| O35            | O                   | 0.70450          | 0.66866          | 0.20291          | 1.0000              |

| C1              | C                   | 0.31163          | 0.44589          | 0.35679          | 1.0000              |
# Kaolinite slab + methanol at SiO2

data_SiO2+M

_symmetry_Int_Tables_number  1
_cell_length_a  10.384527
_cell_length_b  9.011475
_cell_length_c  22.250826
_cell_angle_alpha  90.000000
_cell_angle_beta  90.000000
_cell_angle_gamma  90.000000

loop_{
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1  x,y,z
}

loop_{
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Al1  Al  0.34955  0.47089  0.55292  1.0000
Al2  Al  0.33739  0.80651  0.55226  1.0000
Al3  Al  0.58833  0.97216  0.55153  1.0000
Al4  Al  0.59787  0.30477  0.55258  1.0000
Al5  Al  0.84959  0.47072  0.55322  1.0000
Al6  Al  0.83727  0.80591  0.55265  1.0000
Al7  Al  0.08856  0.97223  0.55199  1.0000
Al8  Al  0.09794  0.30455  0.55286  1.0000
Si1  Si  0.26199  0.31881  0.43025  1.0000
Si2  Si  0.26742  0.64674  0.43099  1.0000
Si3  Si  0.50895  0.81930  0.43005  1.0000
Si4  Si  0.51872  0.14741  0.43012  1.0000
Si5  Si  0.76207  0.31888  0.43029  1.0000
Si6  Si  0.76823  0.64626  0.43126  1.0000
Si7  Si  0.00841  0.81955  0.43081  1.0000
Si8  Si  0.01850  0.14735  0.43042  1.0000
O1  O  0.25044  0.33115  0.50393  1.0000
O2  O  0.28811  0.63702  0.50416  1.0000
O3  O  0.28960  0.48238  0.40186  1.0000
O4  O  0.37418  0.20115  0.41176  1.0000
O5  O  0.37304  0.75923  0.40177  1.0000
O6  O  0.48983  0.83684  0.50348  1.0000
O7  O  0.53460  0.14089  0.50365  1.0000
O8  O  0.60675  0.98184  0.40207  1.0000
O9  O  0.62086  0.69680  0.41740  1.0000
O10 O  0.62669  0.25856  0.40221  1.0000
O11 O  0.24211  0.94516  0.50666  1.0000
O12 O  0.15131  0.13346  0.59892  1.0000
O13 O  0.19536  0.44591  0.59762  1.0000
O14 O  0.17864  0.82003  0.59666  1.0000
O15 O  0.50091  0.44657  0.50727  1.0000
O16 O  0.40646  0.64289  0.59711  1.0000
O17 O  0.42875  0.95814  0.59760  1.0000
O18 O  0.44601  0.32930  0.59951  1.0000
O19 O  0.53310  0.74667  0.28620  1.0000
O20 O  0.75040  0.33127  0.50399  1.0000
O21 O  0.79015  0.63564  0.50446  1.0000
O22 O  0.79041  0.48215  0.40186  1.0000
O23 O  0.87392  0.20046  0.41214  1.0000
O24 O  0.87348  0.75926  0.40212  1.0000
O25 O  0.99098  0.83578  0.50410  1.0000
O26 O  0.03460  0.14058  0.50393  1.0000
O27 O  0.04050  0.98162  0.40230  1.0000
O28 O  0.12105  0.69936  0.41525  1.0000
O29 O  0.12673  0.25782  0.40233  1.0000
O30 O  0.74257  0.94466  0.50671  1.0000
O31 O  0.65107  0.1335  0.59860  1.0000
O32 O  0.69512  0.44573  0.59758  1.0000
O33 O  0.67798  0.81970  0.59641  1.0000
O34 O  0.00125  0.44609  0.50381  1.0000
O35 O  0.90633  0.64258  0.59769  1.0000
References

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