

Silanization of superficially porous silica particles with p-aminophenyltrimethoxysilane

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ABSTRACT

The surface functionalization of silica particles for chromatographic applications is typically achieved by means of silanization reactions. A silane molecule (e.g., chlorosilanes or alkoxysilanes) with a functional group of interest is attached to the silica surface through a siloxane bond. Even though the surface modification via silanization is widely used, how the reaction parameters affect the degree of surface coverage is rarely discussed, particularly when using the less reactive alkoxysilanes reagents. We studied reaction conditions to graft p-aminophenyltrimethoxysilane (p-APTMS) on superficially porous particles. Theoretical calculations predicted that 3 grafts of p-APTMS per nm² (~5 μmol/m²) can be accommodated on the silica surface. This value is not achieved unless the reaction conditions are optimized. To maximize the surface coverage of the aminophenyl layer at the silica surface, we investigated the influence of temperature, reaction time, and addition of water to the silanization reaction on the surface coverage. After optimization, it was found that using elevated temperatures (130 °C),

adding 3.3 equivalents of water per p-APTMS molecule, and reacting for 24 h in decane as the solvent provided a surface coverage as high as $4.5\mu\text{mol}/\text{m}^2$ ($2.7\text{ grafts}/\text{nm}^2$), approaching the limit suggested via theoretical density functional theory calculations.

Keywords: superficially porous particles, silanization, silica surface modification, surface coverage, aminophenyl layer, p-aminophenyltrimethoxysilane, density functional theory

1. Introduction

The modification of inorganic silica with organic functional molecules has been critical to create materials for a variety of applications. In chromatographic as well as in catalytic applications, for example, a functional group is grafted on the silica surface to impart a specific characteristic for a given function, being a stationary phase for chromatography or the group responsible for catalytic action [1,2]. The traditional approach to modify the surface of silica particles is by means of silanization reactions [3]; the surface silanol groups of the silica react with a silane molecule, most typically a chlorosilane, containing the chemical functionality of interest. The result is a silica surface containing the desired functional group anchored through a siloxane bond. In high performance liquid chromatography (HPLC), this functional group acts as the stationary phase. The silanol groups on the silica surface are necessary and they are typically maximized to ensure good anchoring at the silica surface [4]. A fully hydroxylated silica has a total of $8\mu\text{mol}/\text{m}^2$ $-\text{OH}$ groups present on the surface [5]. In many situations, it is desirable to have a high surface coverage to effect retention and improve hydrolytic stability [6].

For chromatographic purposes, residual silanols after anchoring the stationary phase are undesirable, particularly because of the mixed interactions they provide along with the peak

tailing associated with their presence when analyzing basic solutes [7]. The effect of silanols in chromatographic media has been a topic of considerable chromatographic studies [8-10]. We have been interested in developing a dense and rigid layer of aminophenyl groups on silica particles with the purpose of introducing stability and “bulkiness” that may reduce possible undesirable interactions with silanols. The introduction of the amino group should also provide a site to further derivatization, if desired. Having high surface coverage of the ligand ensures minimal amount of residual silanols [11].

Monolayers of aminophenyl groups have been reported for mesoporous silica [12-14]. These materials, however, are different than those used for HPLC and they have been used for a different set of applications (e.g., in sensors, adsorption, catalysis, and drug delivery). In the rare occasion that aminophenylsilane groups have been attached to larger silica particles, the silica gel sizes are still not used for HPLC packing and there has been, basically, no effort to maximize the surface content of aminophenyl groups [15,16].

We investigated the functionalization of superficially porous silica particles with p-aminophenyltrimethoxysilane (p-APTMS) with the goal of achieving a high surface coverage. Our intent was to maximize the number of amino groups at the surface since such a moiety will be used for other functionalization purposes. We point out that a small increase in separation efficiency has been reported when using particles having surface coverage of 3 $\mu\text{mol}/\text{m}^2$ over those with 2 $\mu\text{mol}/\text{m}^2$; however, as stated in the report the pore size difference may contribute to the difference in dispersion that affects efficiency [17]. In our study, we first estimated the number of p-APTMS molecules that can be chemisorbed on the silica surface via theoretical dispersion-corrected density functional theory calculations and then optimized different reaction conditions to maximize the surface coverage. We investigated the influence of temperature,

reaction time, and addition of water on the p-APTMS surface coverage of the superficially porous particles.

2. Materials and methods

2.1 Chemicals

The p-aminophenyltrimethoxysilane (p-APTMS) was purchased from Gelest, Inc. (Morrisville, PA, USA). 5 μm Kinetex superficially porous particles were acquired from Phenomenex (Torrance, CA, USA). Toluene and anhydrous decane were purchased from Sigma-Aldrich (St. Louis, MO, USA). Methanol and acetone were obtained from Fisher scientific (Fair Lawn, NJ, USA). Potassium bromide was purchased from Alfa Aesar (Haverhill, MA, USA). Barnstead International EASYPure II water purifier was used to collect filtered (0.2 μm), deionized (18.2 M Ω cm) water. Nitrogen gas (99.995%) was purchased from PRAXAIR, Inc. (Danbury, CT, USA).

2.2 Computational details

A computational study was undertaken prior to the experimental work. The density functional theory calculations performed made use of both the Vienna Ab initio Simulation Package (VASP) [18] and the Amsterdam Density Functional (ADF) package [19-21] for the periodic and molecular calculations, respectively. Within both software packages, the revised Perdew-Burke-Ernzerhof [22] (revPBE) generalized gradient approximation (GGA) density functional was used with the Grimme3 dispersion correction [23], called revPBE-D3. A plane wave basis set with an energy cutoff of 300 eV was used for all periodic calculations so as to reduce the computational expense for these large silica/p-APTMS models, while a triple zeta basis set with polarization functions (TZP) was used for the molecular calculations [24]. The

projector augmented wave (PAW) method [25,26] for treating the core electrons was used as implemented within VASP, while the core electrons were frozen within the ADF calculations. In both sets of calculations, the Si (3s/3p), O (2s/2p), N (2s/2p), C (2s/2p), and H (1s) electrons were treated explicitly. The k -space consisted of a 1x1x1 Monkhorst-Pack [27] scheme for all periodic calculations since a large unit cell of size 21.40 Å x 21.40 Å x 35.00 Å was employed to model the silica surface. All atoms were allowed to relax fully within the chemisorbed surface-adsorbate systems for all coverages examined, and the silica surface employed in the periodic calculations contained 4.6 OH/nm², which is in accordance with fully hydroxylated silica [28]. The silica surface with 4.6 OH/nm² coordinates was produced based on Comas-Vives work [29]. The geometry optimizations in VASP were performed with a dipole correction applied to the z-axis. Gibbs free energies were calculated using ADF. A test was performed that compared the $\Delta H(\text{rxn})$ computed for the 0.2 p-APTMS/nm² coverage model with an energy cutoff of 500 eV versus that obtained with a 300 eV cutoff. The smaller cutoff was chosen, since it reduced the computational expense for all of the periodic calculations in this study, with the energies being found to be comparable (a difference of less than 1 kcal/mol).

2.3 Silanization

Superficially porous particles (SPPs) were boiled in water for 1 h to maximize the number of -OH groups at the surface. The particles were decanted and dried at 120 °C prior to modification. In this study, the hydrolyzed silica was added to 2.5 mL of anhydrous decane per 100 mg of silica particles in a round bottom flask. Water was added in a 1:2 (silanol:H₂O) molar ratio and the solution was stirred for 1 h. Then, p-APTMS was added in a 1:1.05 (silanol:p-APTMS) molar ratio (i.e., one molecule of p-APTMS reagent per hydroxyl group of a fully hydroxylated silica surface). For the reaction time studies, the reaction was monitored for 5, 12

and 24 h keeping the system under nitrogen and performed at 130 °C. Afterward, the particles were collected and rinsed using toluene, methanol, methanol/water (50:50 v/v) and acetone with 3 cycles of washes and recovery via centrifugation per solvent. Toluene was used to remove decane, methanol is used to remove toluene (methanol is miscible with toluene), the mixture of methanol/water is used to remove unreacted polar reagent and acetone was utilized because of its low boiling point and easily removed from the particles via evaporation. For the temperature studies, the reaction time was kept fixed at 24 h keeping the system under nitrogen and performed at the temperatures of 100, 120 and 130 °C. Then, the particles were collected and rinsed as previously described.

To study the effect of adding water to the silanization reaction, the SPPs were treated and dispersed in decane as above. Reactions with different amount of water were performed having water in a 1:2, 1:4 and 1:10.5 (silanol:H₂O) molar ratio; the solution was stirred for 1 h. Then, p-APTMS was added in a 1:1.05 (silanol:p-APTMS) molar ratio to each reaction and allowed to proceed for 24 h keeping a temperature of 130 °C. Afterwards, the particles were collected and rinsed as previously described.

2.4 Instrumentation

The surface area of the SSP was obtained by the BET method [30] using the NOVA 1200e system from Quantachrome (Boynton Beach, FL, USA). The diffuse reflectance infrared Fourier Transform (DRIFT) spectra were obtained using a Perkin Elmer Spectrum Two FT-IR spectrophotometer (Waltham, MA, USA). Samples were pulverized in a 10% ratio with KBr. Instrument was operated to obtain 300 scans with a resolution of 2 cm⁻¹.

Thermogravimetric analysis (TGA) was performed with a Perkin Elmer TGA 7 to assess the surface coverage of the chemically modified SPPs. Analysis was performed under nitrogen

and air at a flow rate of $95 \text{ mL} \cdot \text{min}^{-1}$ heating from $25 \text{ }^{\circ}\text{C}$ to $100 \text{ }^{\circ}\text{C}$ with a 5 min hold at $100 \text{ }^{\circ}\text{C}$ (rate $20 \text{ }^{\circ}\text{C} \cdot \text{min}^{-1}$), $100 \text{ }^{\circ}\text{C}$ to $150 \text{ }^{\circ}\text{C}$ with a 5 min hold at $150 \text{ }^{\circ}\text{C}$ (rate $10 \text{ }^{\circ}\text{C} \cdot \text{min}^{-1}$), and $150 \text{ }^{\circ}\text{C}$ to $950 \text{ }^{\circ}\text{C}$ (rate $10 \text{ }^{\circ}\text{C} \cdot \text{min}^{-1}$).

A portion of the SPPs submitted to silanization with p-APTMS was also sent to Atlantic Microlab (Norcross, GA, USA; www.atlanticmicrolab.com) for Elemental Analysis (EA). For CHN determination, detection limits are 0.3%. Error limits are $\pm 0.3\%$ for both accuracy and precision [31].

3 Results and discussion

The typical silanization reactions on silica particles for chromatographic applications make use of a chlorosilane as the derivatizing reagent. Even though the surface modification via silanization is conventionally used to prepare silica based chromatographic media, how the reaction parameters affect the degree of surface coverage is rarely discussed. For specific applications, one may need to optimize the reaction to produce an appreciable surface coverage. In the specific case of attaching an aminophenyl group at the surface, one must use p-aminophenyltrimethoxysilane (or another alkoxysilane) as the silanizing reagent since a chlorosilane is not readily available. Alkoxysilanes are less reactive than their chlorosilane counterpart, and therefore, a reaction optimization is necessary to maximize surface coverage. We selected p-APTMS for the silanization reaction of SPPs; a generalized reaction scheme is shown in Fig. 1.

3.1 Computational modeling

Prior to experimentally derivatizing the surface of SPPs with p-APTMS, the selection of the experimental conditions was assisted through a computational investigation of the reaction of

p-APTMS with a silica surface. The intent was to achieve a high surface coverage of aminophenyl groups on the silica particles. Modeling of the reaction, as described in Section 2.2, showed that the chemisorption of p-APTMS molecules is favorable (see Table 1), as evidenced by the change of the energy for the reaction per molecule ($\Delta E(\text{rxn})/\text{molecule}$) for models with 2.0, 2.6, and 3.1 grafts/nm² coverage, which were calculated to be more stable than an individual p-APTMS molecule chemisorbed to the silica surface model employed (0.2 grafts/nm² coverage). Steric repulsion begins to influence the overall stability of the larger coverage models versus the 2.0 grafts/nm² coverage model, with the $\Delta E(\text{rxn})/\text{molecule}$ for the 3.3 grafts/nm² coverage model being less negative than the 0.2 grafts/nm² coverage model by 2.07 kcal/mol. For comparison, the addition of 3 p-APTMS molecules to the 2.0 p-APTMS/nm² coverage model causes only a 0.24 kcal/mol change in the calculated $\Delta E(\text{rxn})/\text{molecule}$.

In the calculations, we assumed that only one of the methoxy groups in each p-APTMS molecule is removed, producing methanol as a byproduct when the siloxane bond forms with silica. It is possible that experimentally, two methoxy groups from one p-APTMS can be involved in the grafting of silica, either reacting with the surface only or reacting with the surface and another p-APTMS molecule. Computationally, however, this becomes very complicated as geometrical considerations increase. Since the main purpose of the computational study was to estimate the effect of temperature on the reaction as it relates to surface coverage, it was assumed that only one methoxy group leaves the p-APTMS as methanol to keep the computational investigation to a minimum, easy to follow, and straightforward. The energetics indicate that attachment of p-APTMS is very favorable at one site. Chemisorption of p-APTMS onto silica producing one methanol molecule is a very stable arrangement indicating favorable reaction conditions at different temperatures (see Fig. S1); the calculations suggest that additional hydrolysis of chemisorbed p-APTMS molecules seems unfavorable (see Fig. S3, positive ΔG). It

has also been reported that under very limited amount of water, a trimetoxysilane reacted with one hydroxy group at the surface eliminating methanol and the other two methoxy groups remained unreacted [32,33]. Further, the IR spectrum (see below) clearly shows a very well-defined and prominent band at 2850 cm^{-1} corresponding to the C-H stretch of the methoxy groups, which is indicative of a large number of methoxy groups at the surface presumably from the very favorable attachment of p-APTMS through one site. The band will decrease in intensity with less methoxy groups and disappears when all methoxy groups are hydrolyzed.

Fig. 2 illustrates the optimized geometry of the model system with 2.6 grafts/nm^2 that contains 12 p-APTMS molecules chemisorbed to silica per unit cell, alongside a side-view of an isolated p-APTMS molecule chemisorbed to the silica surface model. Although high surface coverage is possible (3.3 p-APTMS/nm^2), a coverage model of around 2.0 p-APTMS/nm^2 has the most negative $\Delta E(\text{rxn})$ (see Table 1). The different chemisorption reactions modeled, optimized geometries, as well as the coordinates used for the modeling are provided in the electronic supplementary material.

3.2 Silanization: surface coverage as a function of reaction temperature and time

Silanization of silica with trialkoxysilanes depends on temperature [34], and temperatures around $100\text{ }^{\circ}\text{C}$ are typically used for chromatographic purposes [35]. We decided to study the reaction temperature based on our computational results, which showed that high surface coverage is possible (i.e., 3.3 p-APTMS/nm^2), but a 2.0 p-APTMS/nm^2 is most stable in terms of enthalpy (see Table 1). It was reasoned that an increase in entropy alongside with the higher temperatures may aid increase surface coverage. In order to explore this, reaction temperatures beyond $100\text{ }^{\circ}\text{C}$ were explored. Because of the theoretical modeling, it was then speculated that entropy, alongside high temperatures, might favor reactivity and hence increasing

surface coverage. In order to explore this, a high boiling point solvent (decane) was selected for the silanization reaction to study surface coverage as a function of reaction temperature. The thermal stability of p-APTMS has been reported to be 485 °C, which was determined by thermogravimetric analysis (TGA) with a 25% weight loss of dried hydrolysates [36]. The reaction time was also studied.

The silanization of the SPPs with p-APTMS was performed at three different temperatures (i.e., 100 °C, 120 °C and 130 °C). For these reactions, two molecules of water per silanol were added to the reaction to facilitate hydrolysis of the p-APTMS molecule, assuming a fully hydroxylated silica surface (i.e., 8 $\mu\text{mol}/\text{m}^2$ silanol groups). The surface area of the SPPs was determined to be 107 m^2/g via the BET method [30]. All reactions were performed for 24 h. The silanization of the SPPs with p-APTMS was also performed at three different reaction times (i.e., 5 h, 12 h, and 24 h). All reactions were performed at 130 °C.

TGA was used to estimate the surface coverage of the p-aminophenyl group by means of Eq. 1. Surface area calculations based on TGA have been reported to be within a 4% agreement to those calculated by elemental analysis [37,38].

$$SC = \frac{\%_{loss} - \%_{blank}}{(100 - cf) * SA * MW_L} * 10^6 \quad \text{Eq. 1}$$

In Eq. 1, SC is the surface coverage in $\mu\text{mol}/\text{m}^2$, $\%_{loss}$ is the percentage of weight loss of the modified particles obtained by TGA in the temperature range of 250 °C to 750 °C, $\%_{blank}$ is the percentage of weight loss of the unmodified SPPs obtained by TGA in the temperature range of 250 °C to 750 °C, MW_L is the molecular weight of the ligand, SA is the surface area of the SPPs ($107 \text{ m}^2/\text{g}$) and cf is the correction factor calculated using Eq. 2;

$$cf = [(m_i - m_f)/m_t] * 100 \quad \text{Eq. 2}$$

where m_i is the initial mass of particles used for the analysis, m_f is the mass at 750 °C and m_t is the total mass used. The weight loss was obtained in the range of 250 °C to 750 °C to ensure elimination of decane (boiling point of 174 °C) that may have remained on the particles.

Fig. 3 illustrates the DRIFT spectra of the particles reacted for 24 h at 100 °C and 130 °C. The spectra clearly indicate signature bands that are associated with the p-APTMS functionality, indicating that the modification proceeded. The SPPs exhibit characteristic Si-O-Si bands in the 1100 cm^{-1} -804 cm^{-1} region of the spectrum. Other observed bands associated with the silica backbone are: 3745 cm^{-1} (-OH vibration of a free silanol) and the silica overtones at 1988 cm^{-1} and 1870 cm^{-1} [39-41]. In addition to the prominent bands associated with silica, other distinguishable bands are the aromatic C-H stretch at 3056 cm^{-1} and 3028 cm^{-1} , -OCH₃ bands at 2850 cm^{-1} , N-H bands at 3489 cm^{-1} , 3388 cm^{-1} and 1622 cm^{-1} , and C=C aromatic at 1605 cm^{-1} and 1513 cm^{-1} [42]. The band at 2850 cm^{-1} , attributed to the C-H vibrations of the methoxy groups, is very prominent and indicates that a large number of methoxy groups remained unhydrolyzed, which suggests that polymerization reactions involving p-AMPS are at minimum.

The thermograms of the particles silanized for 24 h at 100 °C, 120 °C and 130 °C are shown in Fig. 4. Table 2 lists the weight loss by TGA and surface coverage for these reaction temperatures. Fig. 5 shows the thermograms for the particles reacted for 5 h, 12 h and 24 h at 130 °C. It can be noticed that the surface coverage of p-aminophenyl groups on SPPs increases as a function of temperature and time. The highest surface coverage was achieved by reacting the SPPs at 130 °C for 24 h, which corresponds to a surface coverage of 3.5 $\mu\text{mol}/\text{m}^2$. Longer reaction times (48 h) did not yield a higher coverage and at higher temperatures (e.g., 170 °C) the integrity of the moiety was compromised.

3.3 Water in the silanization reaction

Although not on silica particles and with a less bulky trimethoxysilane, it has been reported that surface coverage on the silanization of glass slides can improve by a two-step reaction scheme in which water rinses between steps are performed. This brings copious amounts of water in-contact with the silanized slides [32]. The water rinses prior to the second-step silanization via self-assembly was claimed to hydrolyze the non-reacted methoxy groups of the attached silane in the first silanization, providing sites for reaction in the second silanization step. Unfortunately, IR data was not provided to assess the disappearance of the methoxy groups on the surface as a function of the water rinses. The rinses with water prior to the second silanization increased surface coverage by about 30% [32].

In our work, we silanized silica particles with APTMS in one step reaction. Water was added to the reaction solvent and allowed to adsorb onto the hydrophilic silica prior to adding the silane reagent. The solubility of water in decane is extremely low but increases as a function of temperature [43,44] and with silica in solution, most of the water is expected to be adsorbed on the silica particles. In addition, the dissociation of water increases as a function of temperature [45]; therefore, addition of more water to the reaction can further facilitate hydrolysis of p-APTMS to increase reactivity and contribute to improve surface coverage. Hydrolysis of the silane by the added water occurs near the surface reaction site where the water resides. Unlike the silanization of glass slides [32], we controlled the amount of water and the amount of silane added to the reaction. We evaluated the effect of water content in the silanization reaction at three different water levels. Assuming a silanol content $8 \mu\text{mol}/\text{m}^2$ (a fully hydroxylated silica surface), water was added at silanol:H₂O molar ratios of 1:2, 1:4, 1:10.5, and 1:31.5 (silanol:H₂O). These correspond to 0.63, 1.3, 3.3, and 9.9 molecules of water per hydrolysable

methoxy group on a p-APTMS molecule, respectively. The reactions were performed at 130 °C for 24 h, which were the optimal reaction conditions established previously (see section 3.2). The surface coverage of the p-APTMS modified SPPs was determined by means of TGA and using Eq. 2. Table 3 lists the percentage of nitrogen obtained via elemental analysis and the surface coverage of the p-APTMS modified SPPs reacted with the 1:2, 1:4 and 1:10.5 (silanol:H₂O) molar ratios. It can be observed that as the water content increases in the reaction the surface coverage also increases. The highest surface coverage was achieved by reacting the SPPs at 130 °C for 24 h with a 1:10.5 (silanol:H₂O) molar ratio. Under such conditions, a surface coverage of 4.5 μmol/m² was achieved. Higher water content (molar ratio of 1:31.5 silanol:H₂O) did not yield a higher coverage. It was noted that adding as little as one molecule of water per methoxy group on the silane molecule was sufficient to increase surface coverage by about 30%. Because the controlled amount of water is very small and adsorbed onto the silica, hydrolysis in solution is minimized, vertical polymerization is avoided, and the reaction can proceed in one single step.

4 Conclusion

The reaction conditions for the silanization of superficially porous silica particles with p-APTMS were studied in an effort to maximize surface coverage. The silanization reaction at 130 °C for 24 h using a silanol:H₂O molar ratio of 1:10.5 produced the highest surface coverage. Under these conditions, we achieved a surface coverage of about 4.5 μmol/m²; this is equivalent to 2.7 grafts/nm² coverage, which approaches the favorable value predicted via density functional theory calculations. This is a relatively high surface coverage of aminophenyl groups at the surface, which can shield potential interactions of solutes with surface silanol groups. Further, crosslinking of the surface phenyl groups would improve stability of the aminophenyl layer, a subject that is currently under study in our laboratory. The chromatographic performance

of the aminophenyl layer will also be explored in future work. Nevertheless, of unique importance is that our approach provides a high surface coverage of a hydrophobic, protective phenyl layer on the silica surface. At the same time, the amino functionality is incorporated, which allows for further functionalization of the surface to introduce stationary phases with other characteristics.

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Declaration of interest

The authors have declared no conflict of interest.

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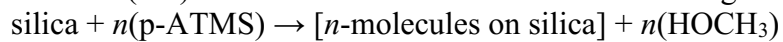
Highlights:

- The reaction of p-aminophenyl trimethoxysilane (p-APTMS) on superficially porous silica particles was studied.
- Reaction temperature, time, and water content in the reaction were optimized to maximize surface coverage.
- Computational calculations predicted a p-APTMS surface coverage of approximately 5 $\mu\text{mol}/\text{m}^2$.
- Optimized reaction conditions resulted in a surface coverage of $\sim 4.5 \mu\text{mol}/\text{m}^2$.

Table 1. The surface coverage (molecules/nm²), number of p-APTMS molecules chemisorbed to silica, and the ΔE of the reaction per molecule for different modeled systems.

p-APTMS/nm ²	p-APTMS count (<i>n</i>)	$\Delta E(\text{rxn})/\text{molecule (kcal/mol)}^a$
0.2	1	-9.51
2.0	9	-20.06
2.6	12	-19.82
3.1	14	-11.61
3.3	15	-7.44

^a The $\Delta E(\text{rxn})/\text{molecule}$ was calculated for the following reaction:



via $\Delta E(\text{rxn})/\text{molecule} = [n \times E(\text{methanol}) + E(n\text{-molecules on silica}) - E(\text{silica}) - n \times E(\text{p-APTMS})]/n$

Table 2. Surface coverage of p-APTMS for the reactions carried out at 100 °C, 120 °C and 130 °C for 24 h based on weight loss via TGA.

Reaction Temperature	Weight loss (%) ^a	Surface Coverage (μmol/m ²) ^b
100 °C	3.24	2.6
120 °C	3.65	3.0
130 °C	3.97	3.4

^a Weight loss in the temperature range of 250 °C to 750 °C (for unmodified SPPs was 0.77%).

^b Calculations were performed using equation 1. The error associated with the surface coverage is $\pm 0.1 \mu\text{mol/m}^2$.

Table 3. Surface coverage of p-APTMS for the reactions based on weight loss via TGA for p-APTMS modified SPPs at different silanol:water molar ratio in the silanization reaction.

silanol:water molar ratio	Weight loss (%) ^a	Surface Coverage ($\mu\text{mol}/\text{m}^2$) ^b
1:2	4.06	3.4
1:4	3.99	3.3
1:10.5	4.86	4.3
1:31.5	5.00	4.4

^a Weight loss in the temperature range of 250 °C to 750 °C (for unmodified SPPs was 0.77%).

^b Calculations were performed using equation 1. The error associated with the surface coverage is $\pm 0.1 \mu\text{mol}/\text{m}^2$.

Figure Captions

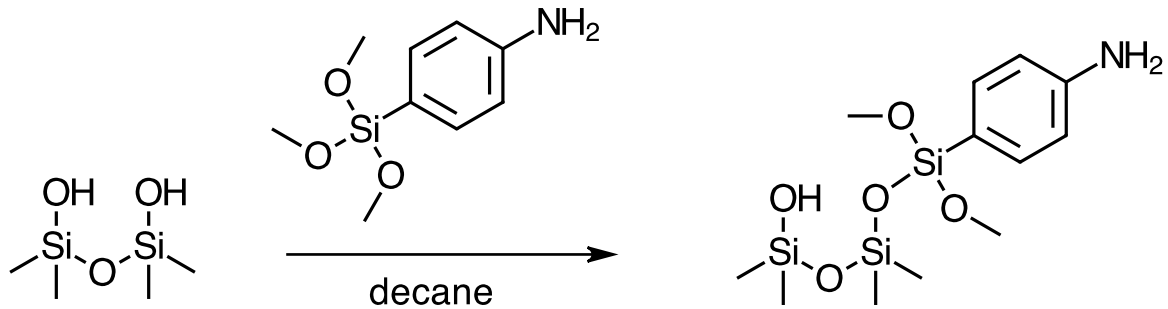
Fig. 1. Schematic representation of the reaction between silica and p-APTMS using decane as solvent.

Fig. 2. Optimized geometries of: (A) the top-left quadrant of a model system with 2.6 grafts/nm², which contains 12 p-APTMS molecules chemisorbed to silica per unit cell, (B) the 2.6 p-APTMS/nm² coverage model, which contains 12 p-APTMS molecules chemisorbed to silica per unit cell, (C) the 0.2 p-APTMS/nm² coverage model, being a chemisorbed p-APTMS monomer. The grey color depicts the carbon atoms in the system, red represents the oxygen atoms, blue the nitrogen atoms, white shows the hydrogen atoms, and turquoise illustrates the silica atoms.

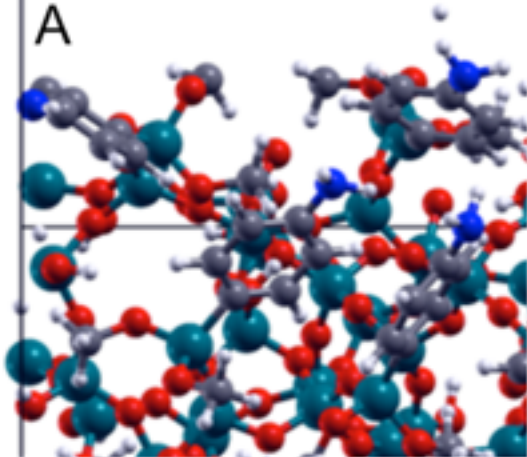
Fig. 3 DRIFT spectra of the particles reacted with p-APTMS for 24 h at 100 °C and 130 °C normalized to the minimum reflectance of each spectrum. The spectra have been shifted for clarity.

Fig. 4. Thermograms illustrating the weight percent loss as a function of temperature in the range of 250-750 °C for the silica particles reacted with p-APTMS at 130 °C for 5 h ($\Delta Y = 2.70\%$), 12 h ($\Delta Y = 3.42\%$) and 24 h ($\Delta Y = 3.97\%$). The thermogram corresponding to unmodified silica ($\Delta Y = 0.77\%$) is also included for comparison.

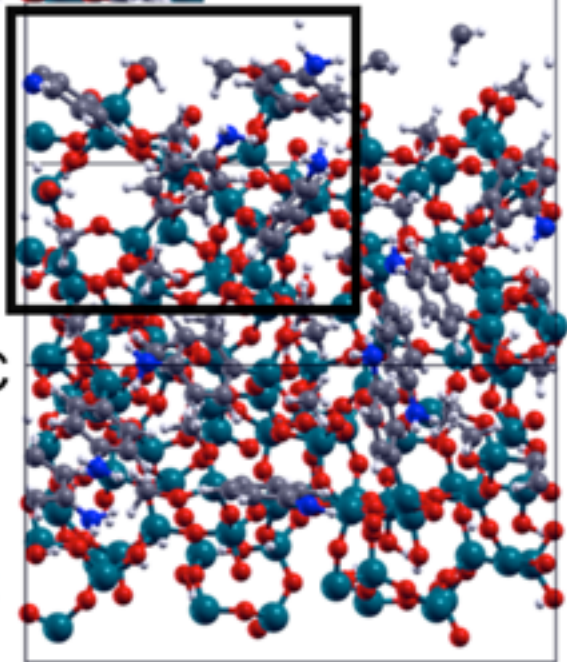
Fig. 5. Thermograms illustrating the weight percent loss as a function of temperature in the range of 250-750 °C for the particles reacted with p-APTMS for 24 h at 100 °C ($\Delta Y = 3.24\%$), 120 °C ($\Delta Y = 3.65\%$) and 130 °C ($\Delta Y = 3.97\%$). The thermogram corresponding to unmodified silica ($\Delta Y = 0.77\%$) is also included for comparison.



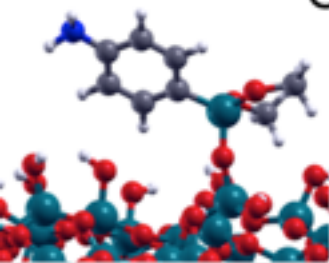
A

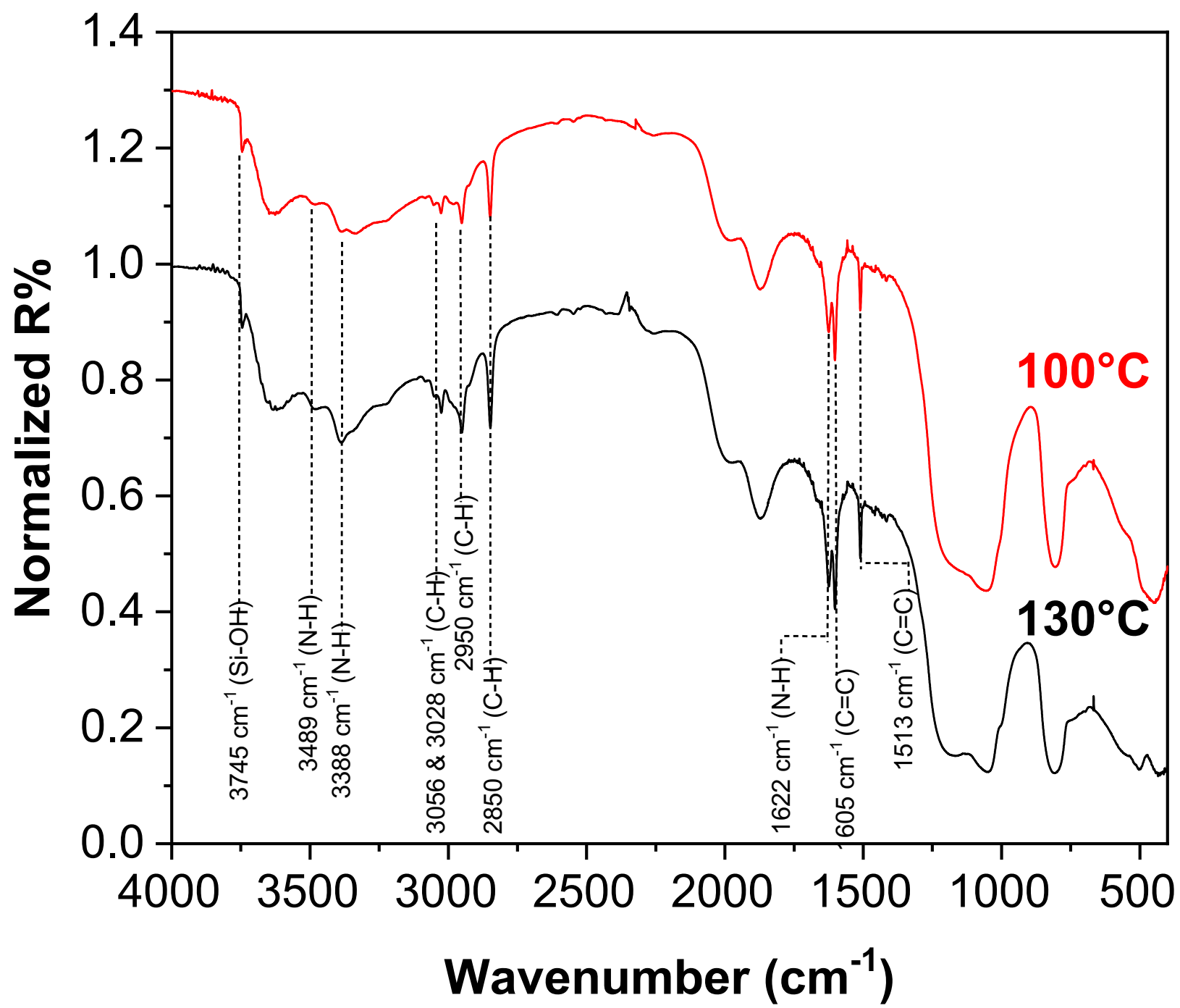


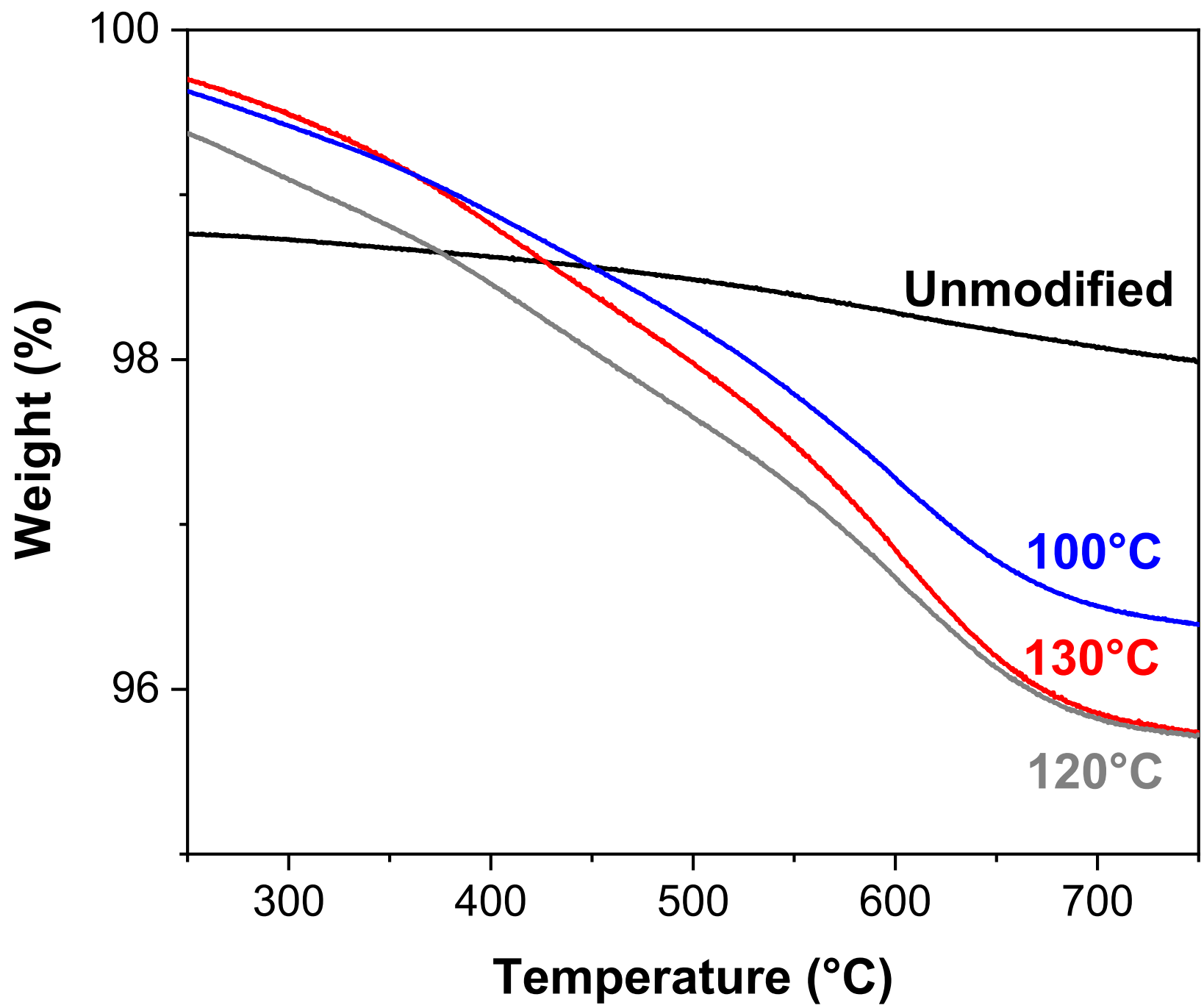
B

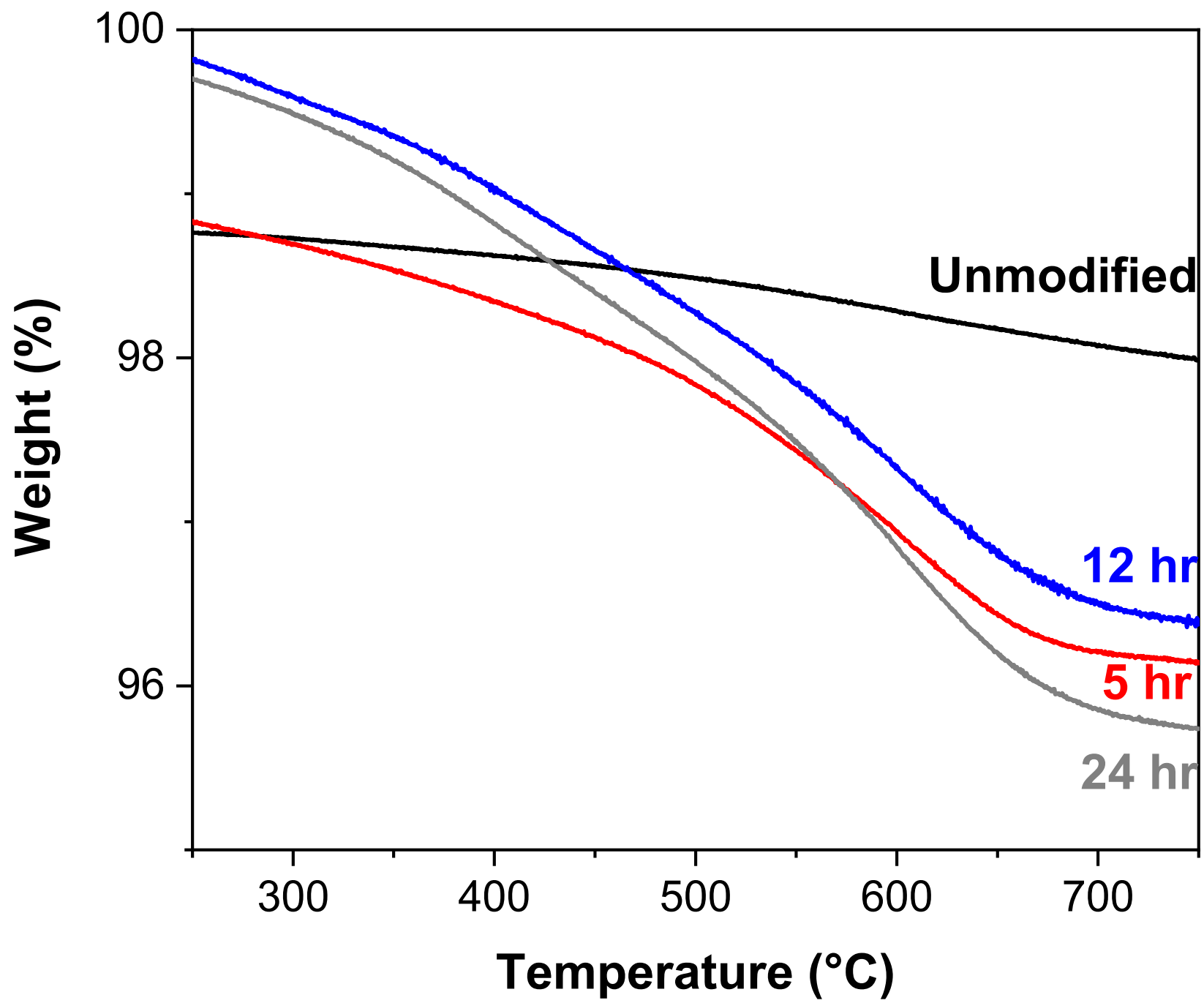


C









Silanization of superficially porous silica particles with p-aminophenyltrimethoxysilane

Supplementary Material

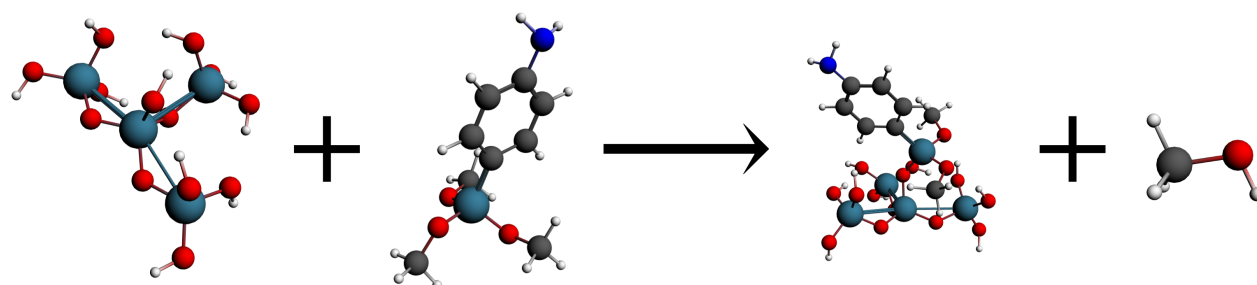
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Section 1. Chemisorption of p-Aminophenyltrimethoxysilane (p-APTMS) to a Silica Cluster.....	S2
Section 2. Reactions Involving Two p-APTMS Molecules (Hydrolysis)	S3
Section 3. Chemisorption of p-APTMS to Silica (4.6 OH/nm ²) with Modeled Coverages of 0.2, 2.0, 2.6, 3.1 and 3.3 p-APTMS/nm ²	S4-S8
Section 4. Coordinates (XYZ and POSCAR Format).....	S9-S93

Section 1.

Chemisorption of p-Aminophenyltrimethoxysilane (p-APTMS) to a Silica Cluster – Molecular Calculations with ADF Software Package



$$\Delta G = \sum \Delta G (\text{products}) - \sum \Delta G (\text{reactants})$$

T = -273.15 °C	-16.6 kcal/mol
T = 25 °C	-10.2 kcal/mol
T = 151.85 °C	-7.6 kcal/mol
T = 169.85 °C	-7.2 kcal/mol
T = 189.85 °C	-6.8 kcal/mol

Fig. S1. The difference in Gibbs Free Energy between a Silica cluster plus a p-APTMS versus a chemisorbed p-APTMS-Silica cluster plus a methanol. The entropy stabilizes the separated Silica cluster and p-APTMS when temperature is increased, but the chemisorbed p-APTMS-Silica cluster plus a methanol remains the most stable system until approximately 510 °C is reached.

Section 2.

Reactions Involving Two p-APTMS Molecules (Hydrolysis) – Molecular Calculations with ADF Software Package

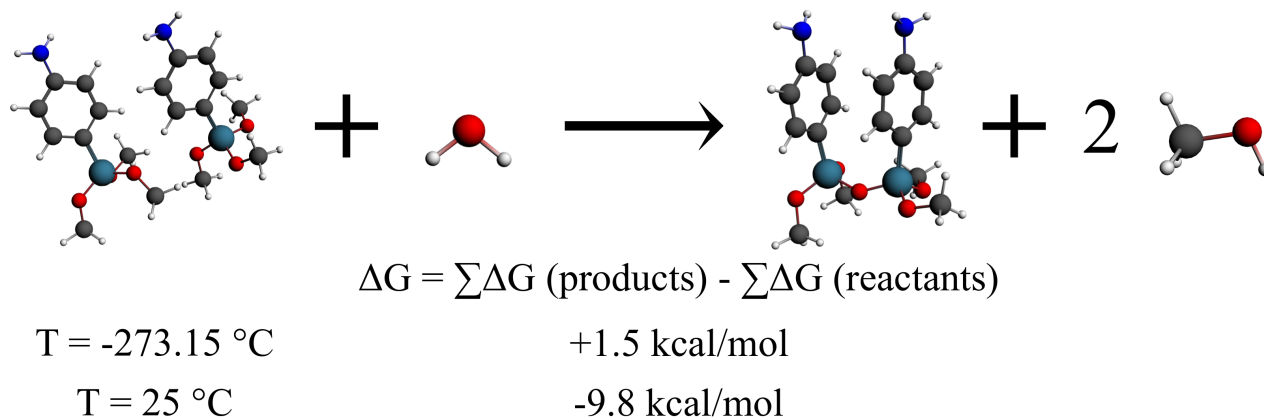


Fig. S2. The difference in Gibbs Free Energy between two p-APTMS molecules plus water versus a hydrolyzed p-APTMS dimer cluster plus two methanol molecules.

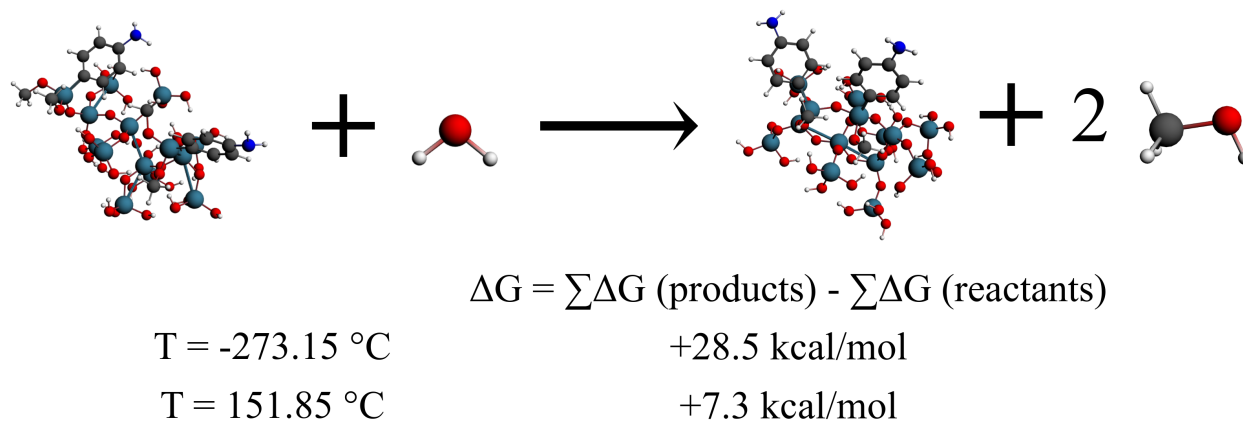


Fig. S3. Similar to Fig. S2, but for the hydrolysis of two p-APTMS molecules while chemisorbed to silica. The hydrolysis of chemisorbed p-APTMS molecules is unfavorable, even at high temperatures, but this is most likely because a second methoxy group from each molecule must be broken off and has oxygen holding the two molecules together, while also being attached to the substrate, resulting in strained bonds within the system.

Section S3.

Chemisorption of p-APTMS to Silica (4.6 OH/nm^2) with Modeled Coverages of 0.2, 2.0, 2.6, 3.1 and 3.3 p-APTMS/nm^2 – Periodic Calculations with VASP Software Package

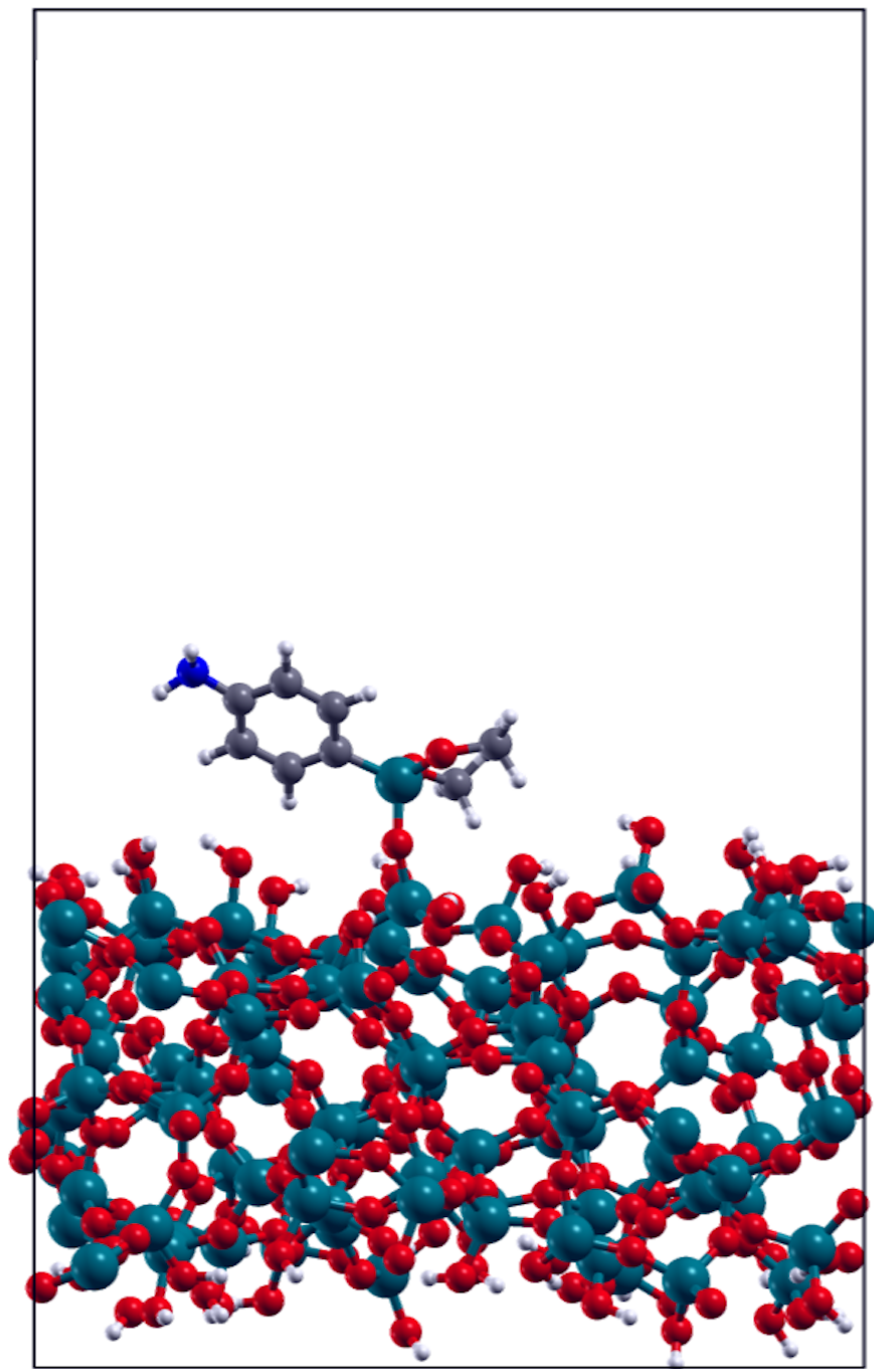


Fig. S4. Optimized geometry of the 0.2 p-APTMS/nm^2 coverage model, which contains 1 p-APTMS molecule chemisorbed to silica per unit cell.

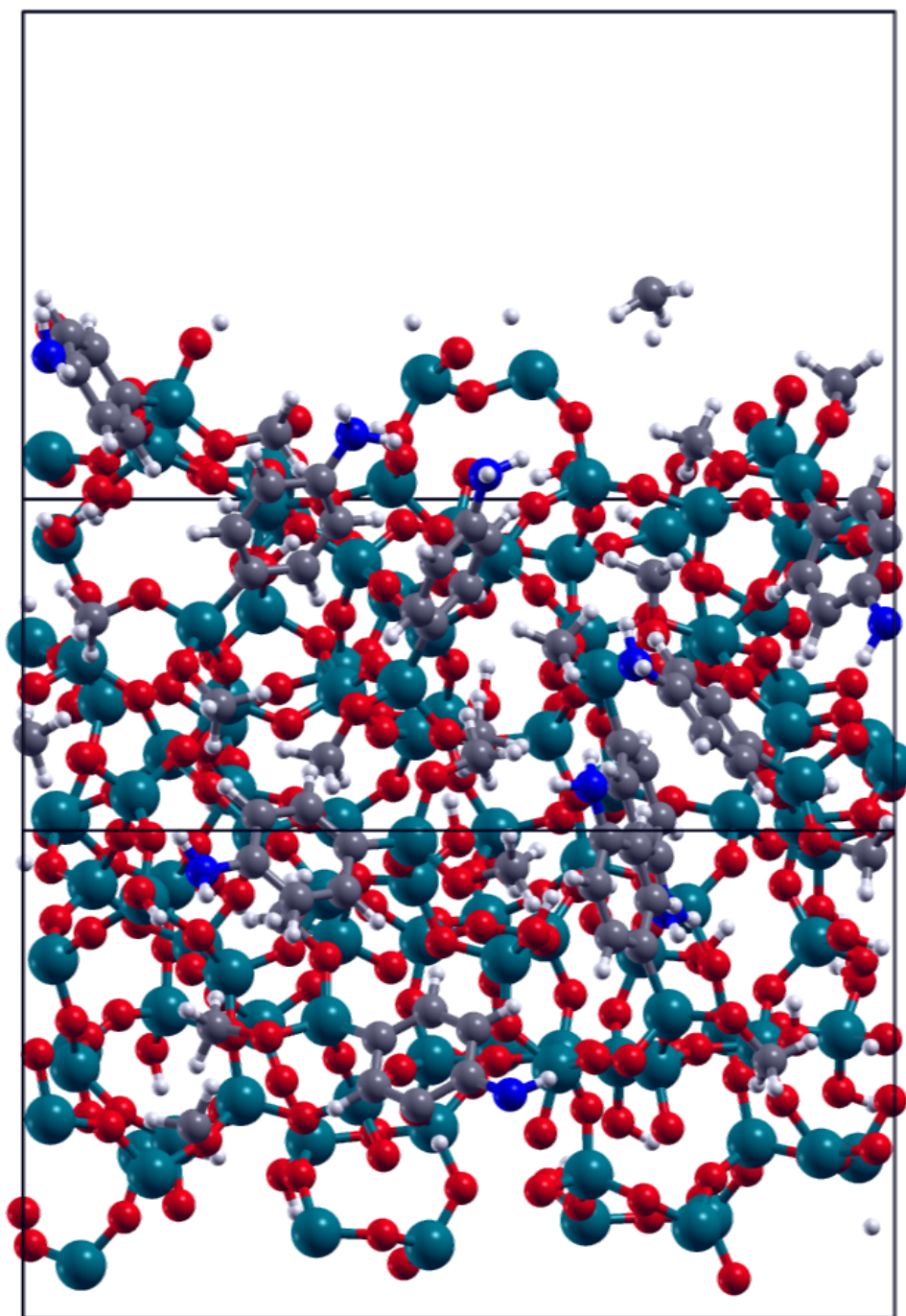


Fig. S5. Optimized geometry of the 2.0 p-APTMS/nm² coverage model, which contains 9 p-APTMS molecules chemisorbed to silica per unit cell. The "lone" atoms are bonded to other atoms in the neighboring unit cells, and hence their bonds are not shown.

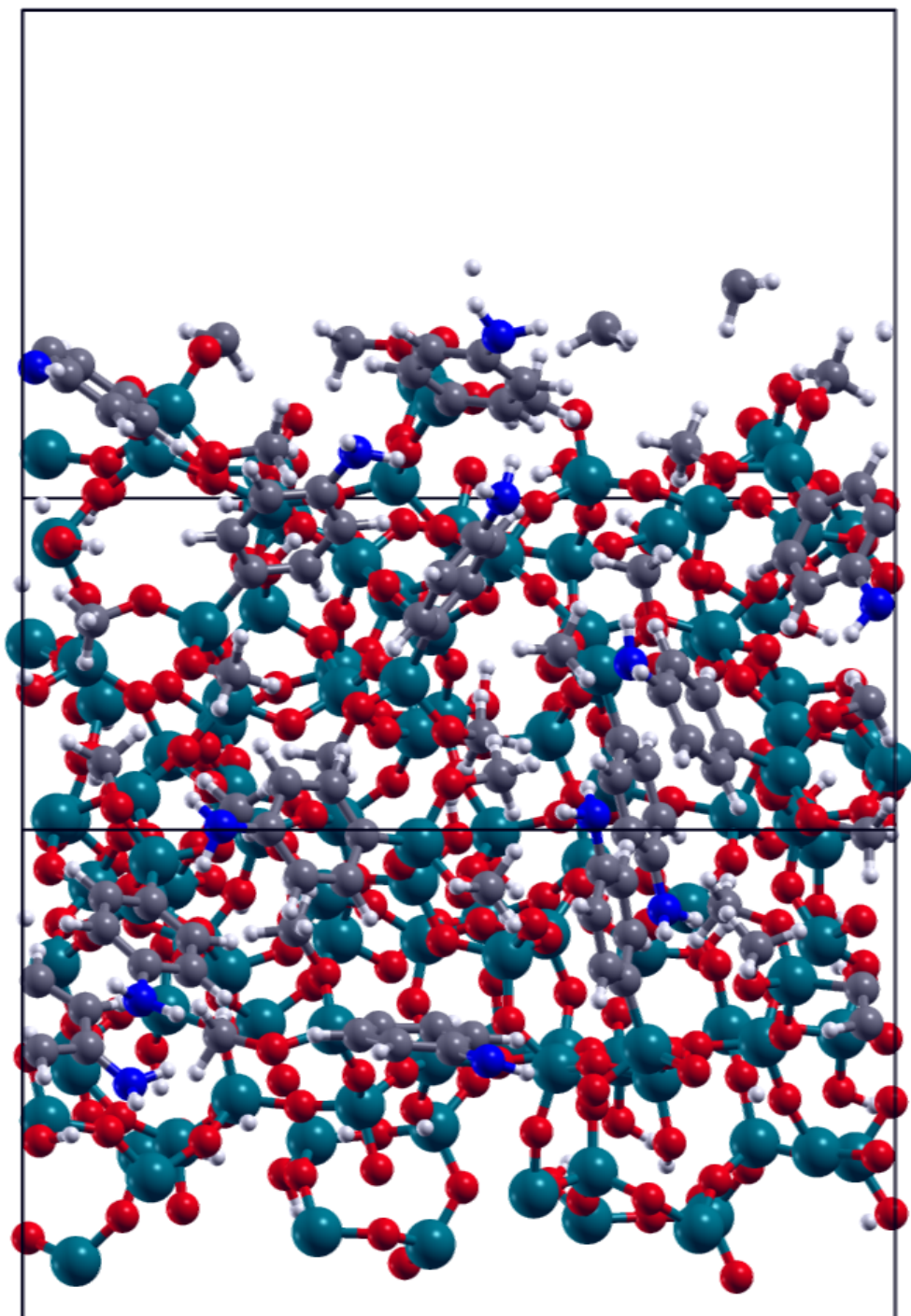


Fig. S6. The optimized geometry of the 2.6 p-APTMS/nm² coverage model, which contains 12 p-APTMS molecules chemisorbed to silica per unit cell. The "lone" atoms are bonded to other atoms in the neighboring unit cells, and hence their bonds are not shown.

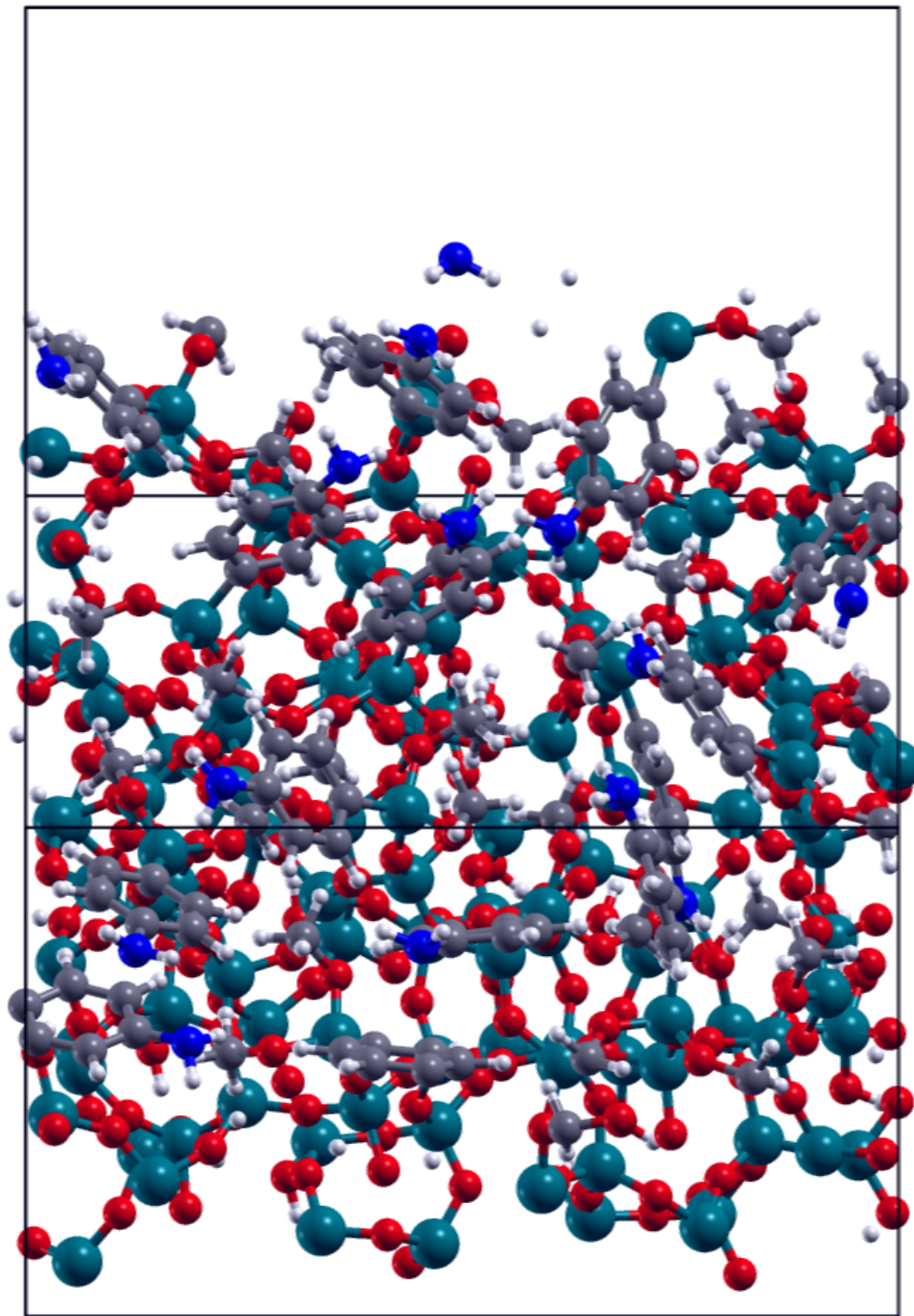


Fig. S7. The optimized geometry of the 3.1 p-APTMS/nm² coverage model, which contains 14 p-APTMS molecules chemisorbed to silica per unit cell. The "lone" atoms are bonded to other atoms in the neighboring unit cells, and hence their bonds are not shown.

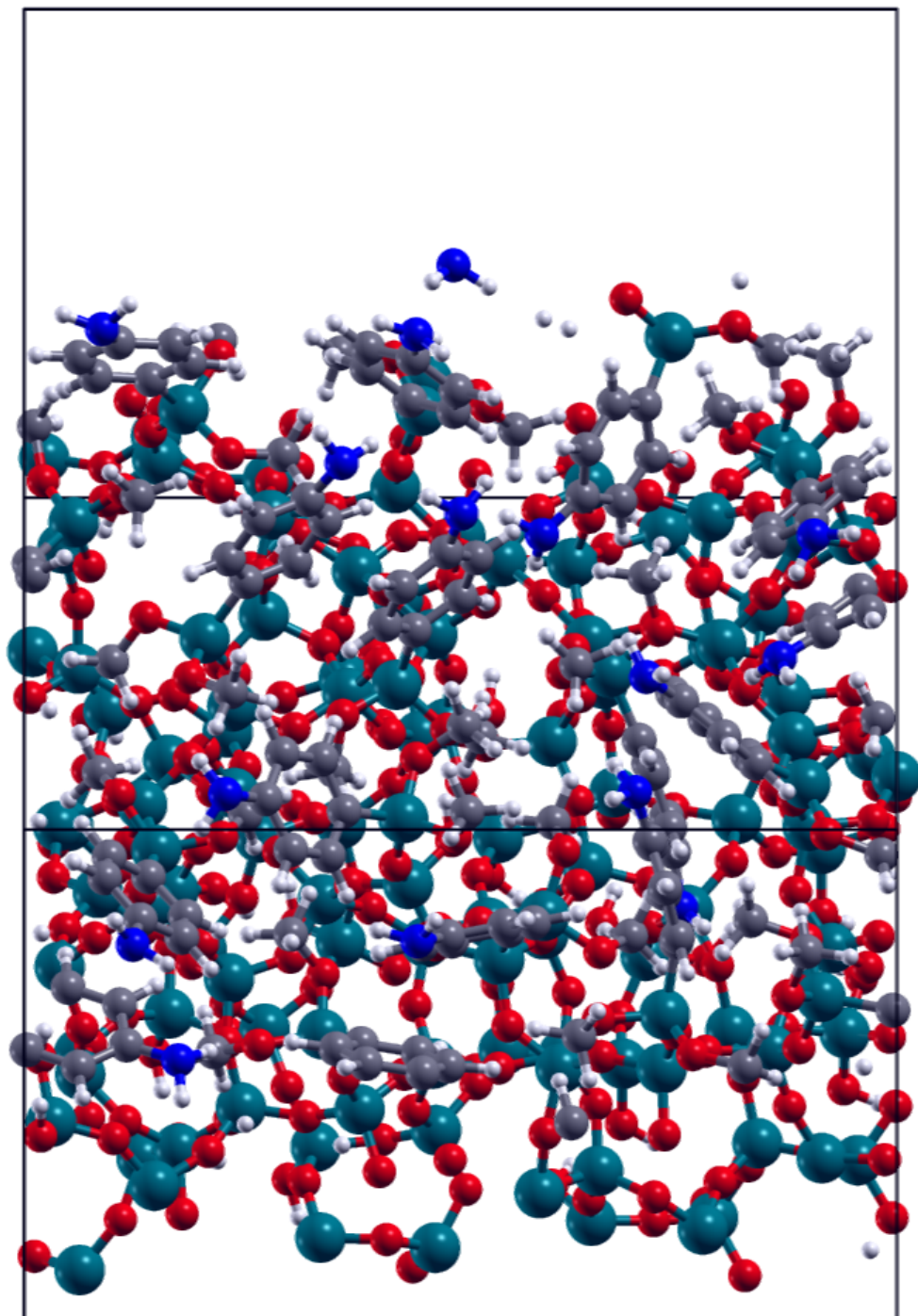


Fig. S8. The optimized geometry of the 3.3 p-APTMS/nm² coverage model, which contains 15 p-APTMS molecules chemisorbed to silica per unit cell. The "lone" atoms are bonded to other atoms in the neighboring unit cells, and hence their bonds are not shown.

Section S4.

Coordinates (XYZ and POSCAR Format)

Methanol:

O -0.453398 0.364939 0.000000
C -1.879368 0.150582 0.000000
H -0.031251 -0.512035 0.000000
H -2.345567 1.145079 0.000000
H -2.219788 -0.394071 -0.899855
H -2.219788 -0.394071 0.899855

p-APTMS:

Si -0.120126 -0.634225 -0.767944
O -0.305722 -2.023252 0.118829
O 1.466353 -0.155700 -0.624199
O -0.998994 0.656665 -0.172640
N -1.792982 -1.714804 -6.556229
C -0.759917 -2.316785 -3.023375
C -1.121305 -2.554859 -4.352235
C -1.380845 -1.478471 -5.229863
C -1.284472 -0.160760 -4.729829
C -0.928590 0.063154 -3.397180
C 1.912488 1.044440 -1.288631
C 0.120609 -2.055994 1.499326
C -0.649506 -1.003916 -2.511135
C -2.441416 0.622310 -0.200006
H -1.472835 -2.603764 -6.934484
H -1.576166 -0.954341 -7.196858
H -1.495175 0.684504 -5.392059
H -0.871348 1.095057 -3.038736
H -1.206719 -3.581732 -4.721383
H -0.562289 -3.168976 -2.368649
H 1.220024 -2.056460 1.568064
H -0.269938 -1.192456 2.063500
H -0.271340 -2.979628 1.949074
H 1.809056 0.952850 -2.383792
H 1.343339 1.925113 -0.945656
H 2.974935 1.188110 -1.044637
H -2.805883 1.578533 0.203027
H -2.819688 0.496623 -1.228209
H -2.835000 -0.199446 0.422059

Silica Cluster:

Si -1.089607 0.967646 -2.661246
Si 1.629710 0.642545 0.532285
Si -1.673258 -1.945936 2.289882
Si -1.196975 -0.172545 0.014718

O -0.065493 -1.900482 2.761007
O -2.516507 -0.879777 3.216572
O -2.167257 -3.499738 2.535022
O 1.065052 2.212110 0.537069
O 1.921188 0.151033 2.071467
O 2.996888 0.549772 -0.391889
O -0.508387 2.401498 -2.016090
O 0.188007 0.142533 -3.290633
O -2.170474 1.384320 -3.833187
O -1.856871 0.070226 -1.477992
O -1.811307 -1.552374 0.670811
O -1.572842 1.052907 1.079675
O 0.449053 -0.299216 -0.194591
H 0.419771 -2.702826 2.497456
H -2.464022 0.027604 2.855849
H -3.053003 -3.707564 2.191871
H 1.245793 -0.473892 2.420164
H 0.786863 2.492817 -0.362299
H 3.692360 -0.003855 0.001833
H -2.745704 0.660477 -4.134536
H 0.730287 -0.286193 -2.601593
H -1.216013 3.051936 -1.857458
H -0.867049 1.736447 1.108127

Silica+p-APTMS Model:

Si -1.899033 1.581027 -2.650361
Si 1.818716 0.342692 -0.054695
Si -1.881432 2.442890 1.621232
Si -1.710167 -1.290832 2.353970
Si -1.138997 0.067538 -0.227967
O -3.363524 1.781688 1.995008
O -1.086431 2.286651 3.087678
O -0.377132 -0.441113 2.894778
O -3.073367 -0.864732 3.173559
O -1.332828 -2.874294 2.602372
O 1.735885 1.855125 -0.782737
O 1.987962 0.415865 1.579578
O 3.148851 -0.373196 -0.737909
O -3.005162 2.679437 -2.092191
O -0.395794 2.263661 -2.761901
O -2.465168 1.133667 -4.136683
O -1.885494 0.210998 -1.682362
O -1.952594 -0.999438 0.720806
O -1.068678 1.571171 0.469922
O 0.417767 -0.440343 -0.454210
N -2.115604 8.166240 -0.467516
C -2.859284 5.126776 1.545027
C -2.899439 6.442421 1.081390

C -2.044283 6.861673 0.034127
C -1.159800 5.916592 -0.537151
C -1.121641 4.605420 -0.059219
C 0.187302 2.980456 3.262858
C -4.335563 1.586678 0.918306
C -1.970968 4.176040 0.990038
H -2.473063 8.859625 0.184246
H -1.276326 8.490953 -0.940538
H -0.421172 3.901553 -0.513328
H -0.499430 6.218329 -1.355509
H -3.534750 4.834763 2.353801
H -3.598613 7.158270 1.523507
H -4.096990 2.194578 0.034430
H -4.339032 0.525599 0.630397
H -5.322117 1.873111 1.306222
H 0.972812 2.502804 2.658300
H 0.091466 4.039917 2.981157
H 0.447958 2.908893 4.326843
H -0.640543 0.471111 3.176666
H -3.351327 0.050575 2.942326
H -1.863055 -3.495256 2.075920
H 1.215201 0.031504 2.064133
H 2.579250 2.093622 -1.206122
H 3.587979 -0.998152 -0.135646
H -2.058110 0.317614 -4.472470
H 0.269062 2.061398 -2.069415
H -2.589107 3.455485 -1.672355

Two p-APTMS Molecules:

Si -2.953315 -3.157406 -3.710424
Si 0.505239 -3.124027 0.928332
O 0.484239 -3.940836 -0.519117
O -1.641517 -4.035127 -4.262960
O -4.291031 -3.879387 -4.378025
O -0.569500 -3.912819 1.922933
O -2.926039 -3.179864 -2.040573
O 1.997025 -3.203618 1.673939
N -2.834123 2.744933 -5.324851
N -1.096349 2.709758 0.028514
C 0.614014 -5.377613 -0.552097
C -2.768034 -4.421412 -1.319526
C -1.956064 -0.493288 -3.701311
C -1.906055 0.852705 -4.072469
C -2.847083 1.375366 -4.985996
C -3.839322 0.512056 -5.502162
C -3.881137 -0.832257 -5.119470
C -0.312730 -3.621380 -3.869087
C -4.417050 -5.313055 -4.468755

C -2.942864 -1.369531 -4.208883
C -0.908579 -3.348336 3.208628
C 3.168086 -2.767165 0.952209
C 0.045232 -1.353269 0.615042
C 0.703243 -0.301003 1.294475
C 0.323818 1.033865 1.123061
C -0.745093 1.365501 0.260364
C -1.027176 -1.005112 -0.240296
C -1.416415 0.323929 -0.416880
H 1.560484 -5.706651 -0.091530
H -0.223786 -5.862560 -0.025978
H 0.602685 -5.686456 -1.607438
H -3.750064 -4.896527 -1.159416
H -2.110831 -5.122915 -1.858373
H -2.312362 -4.198344 -0.345213
H -1.912129 3.171245 -5.255675
H -3.247876 2.943276 -6.233612
H -4.580409 0.904309 -6.205710
H -4.658958 -1.476972 -5.535634
H -1.136974 1.506271 -3.649219
H -1.211441 -0.854805 -2.991644
H -0.236704 -3.467095 -2.781425
H 0.386876 -4.418142 -4.162460
H -0.026193 -2.691539 -4.388303
H -3.499428 -5.773200 -4.868922
H -4.637314 -5.753141 -3.481359
H -5.254776 -5.535124 -5.146122
H 3.522243 -3.557040 0.268865
H 2.973411 -1.854746 0.363368
H 3.957291 -2.549119 1.687135
H -0.070308 -3.453310 3.917237
H -1.173448 -2.280959 3.118947
H -1.777856 -3.898071 3.597714
H -0.882399 3.333073 0.804082
H -2.058845 2.834086 -0.279054
H 1.527581 -0.529077 1.975808
H 0.855133 1.828783 1.655900
H -1.578193 -1.776722 -0.780560
H -2.240597 0.561552 -1.094360

Water:

O 0.000000 0.000000 1.560432
H 0.000000 -0.763581 0.956145
H 0.000000 0.763581 0.956145

Hydrolyzed p-APTMS Molecules:

Si -1.676780 -3.104724 -3.261035

Si -1.074864 -2.977525 -0.216090
O -0.163569 -3.455847 -3.871914
O -2.891618 -3.989920 -3.968672
O -2.180007 -3.481070 0.912820
O -1.688717 -3.533008 -1.650440
O 0.385275 -3.700960 0.127783
N -2.725769 2.884133 -3.713720
N -0.489167 3.110480 -0.491126
C -0.924288 -0.380825 -3.648961
C -1.159577 0.992584 -3.732022
C -2.479400 1.491782 -3.733290
C -3.552496 0.576531 -3.675689
C -3.305718 -0.796489 -3.590716
C 0.320665 -4.812109 -3.815905
C -3.234151 -5.320477 -3.530591
C -1.988670 -1.307495 -3.565012
C -2.070639 -3.031368 2.279327
C 1.498388 -3.627162 -0.783659
C -0.883260 -1.125067 -0.206096
C 0.365759 -0.489080 -0.033372
C 0.497894 0.902402 -0.094359
C -0.631232 1.715335 -0.327000
C -2.009012 -0.291039 -0.408146
C -1.893744 1.097718 -0.464146
H -1.944102 3.432157 -4.068896
H -3.583508 3.146952 -4.196405
H -4.581355 0.950193 -3.683056
H -4.154702 -1.483473 -3.540006
H -0.318774 1.691647 -3.769151
H 0.108221 -0.737215 -3.638660
H 0.045222 -5.307872 -2.869721
H -0.077183 -5.399888 -4.659252
H 1.418224 -4.788536 -3.887080
H -2.500232 -6.057302 -3.898703
H -3.280966 -5.384065 -2.431802
H -4.219960 -5.568837 -3.950439
H 1.771152 -4.643714 -1.107434
H 1.275262 -3.027711 -1.680439
H 2.360722 -3.179414 -0.264285
H -1.263606 -3.566931 2.806474
H -1.876260 -1.946581 2.333050
H -3.027223 -3.245574 2.778135
H 0.265180 3.510988 0.063369
H -1.354464 3.624777 -0.338911
H 1.260094 -1.086839 0.154202
H 1.481853 1.366806 0.027131
H -2.998288 -0.735274 -0.546115
H -2.776681 1.714428 -0.654576

Two p-APTMS Molecules on Silica:

Si -3.009119 8.107482 -11.848293
Si 1.102664 0.377306 -8.792902
Si -3.110921 0.874568 -7.776476
Si -0.702232 2.610767 -7.708847
Si 2.869932 2.824103 -5.987518
Si -2.001468 5.731441 -4.214829
Si -0.786880 1.364019 -3.602614
Si 0.125669 3.781524 -4.970333
Si 2.041855 6.682335 -7.755351
Si -3.647351 5.164907 -8.335358
Si -0.538736 2.748009 -12.157715
Si 1.690564 6.637228 -12.159712
Si -0.624485 5.392967 -8.649189
Si -1.130010 5.734615 -11.762845
O -4.397118 7.921918 -10.918282
O 2.341147 8.172058 -8.386963
O 2.544700 6.759457 -6.194373
O 2.879102 5.482584 -8.559756
O -4.291668 4.262638 -7.091376
O -4.504120 6.547370 -8.521814
O -3.689356 4.336643 -9.764895
O 1.952576 -0.752730 -7.960103
O 0.068895 -0.348860 -9.874196
O 2.035391 1.388664 -9.726353
O -4.663214 1.388562 -7.631999
O -2.893351 -0.292982 -8.942638
O -2.511877 0.149061 -6.413396
O -3.005489 4.366212 -4.406532
O -0.563986 0.627601 -2.146821
O -2.404913 1.581615 -3.943487
O -0.043775 0.383532 -4.718967
O 2.979114 2.980121 -7.625008
O 4.327354 3.255893 -5.347740
O 2.525052 1.256485 -5.606615
O -2.216141 2.219881 -8.202314
O 0.257865 1.284325 -7.695292
O -0.116590 3.808735 -8.665746
O -0.803205 3.104549 -6.143175
O -0.027292 2.847618 -3.609924
O -0.462607 5.277985 -4.653549
O 1.705777 3.899514 -5.407843
O -3.341129 8.833781 -13.296777
O -2.656108 6.855872 -5.219368
O 0.417118 6.318397 -7.794009
O -2.072258 5.512766 -7.895114
O 2.669605 6.735314 -13.488300

O 1.800188 8.015891 -11.230857
O 2.280710 5.403423 -11.227741
O -1.355388 1.757466 -11.123859
O -0.544284 2.090203 -13.677734
O 1.040989 3.036153 -11.694006
O -1.369700 4.169766 -12.171171
O -0.707957 5.928474 -10.187922
O -2.513284 6.545382 -12.098478
O 0.127091 6.366435 -12.645479
N -1.985959 7.620425 1.583650
N 1.382947 11.107250 -8.877849
C -5.136515 9.130213 -10.580761
C -1.918079 7.981867 -5.750664
C -2.777159 7.400234 -2.046253
C -2.772286 7.846165 -0.723106
C -1.962875 7.206583 0.243863
C -1.172708 6.102542 -0.155932
C -1.184418 5.666936 -1.481519
C -4.339692 4.465817 -3.798857
C -1.983659 6.305155 -2.459814
C -0.930056 10.073675 -11.617473
C 0.097884 10.739820 -10.939362
C 0.340089 10.482658 -9.567216
C -0.517872 9.582290 -8.889926
C -1.542882 8.932449 -9.571595
C -4.183286 8.153732 -14.261241
C -1.761269 9.140205 -10.956918
H -5.992786 8.826977 -9.964758
H -4.504232 9.827157 -10.008260
H -5.497019 9.631034 -11.492085
H -1.689576 8.709602 -4.954866
H -0.987649 7.645018 -6.225808
H -2.555209 8.457812 -6.507644
H 2.511517 1.997454 -9.100098
H -0.735981 -0.704556 -9.440358
H 2.365951 -0.377520 -7.155066
H 2.248321 5.999823 -5.659531
H 2.195946 8.197195 -9.361499
H 2.703204 5.456024 -9.540749
H -3.726315 4.290648 -6.288432
H -4.462254 6.928700 -9.434384
H -3.165144 3.513776 -9.750651
H -3.061558 0.068346 -9.833738
H -2.775050 0.610134 -5.583046
H -4.700433 2.365731 -7.497075
H -2.255109 8.591376 1.722058
H -1.148065 7.390812 2.112297
H -0.550750 4.821596 -1.762281

H -0.542841 5.596884 0.582312
H -3.403241 7.919489 -2.776654
H -3.392119 8.698485 -0.429003
H -4.256287 4.700627 -2.728300
H -4.928649 5.239873 -4.311761
H -4.830135 3.492929 -3.930342
H -1.097179 1.000606 -1.424938
H -2.594020 2.529092 -4.160314
H -0.604721 0.203545 -5.505064
H 4.421684 3.064843 -4.399259
H 2.970154 3.928563 -7.958810
H 1.600724 1.014544 -5.354752
H 2.097471 11.504856 -9.483802
H 1.808700 10.501009 -8.175924
H -2.170926 8.228738 -9.019798
H -0.342634 9.377461 -7.832890
H -1.077735 10.269695 -12.682481
H 0.741049 11.443443 -11.476097
H -5.198738 8.000866 -13.860407
H -4.242503 8.788182 -15.155968
H -3.758447 7.175593 -14.536324
H 0.990418 8.570106 -11.247460
H 2.491980 7.494930 -14.067389
H 1.859482 4.519170 -11.425652
H 1.383920 2.418432 -10.990799
H 0.252284 2.304815 -14.191496
H -0.843138 0.962687 -10.845272

Hydrolyzed p-APTMS Molecules on Silica:

Si -2.321412 7.267148 -8.908775
Si 2.966865 1.275864 -8.045267
Si -2.340943 -0.851454 -7.934074
Si -0.134426 1.234715 -7.643704
Si 1.840449 1.948356 -3.935504
Si -1.805439 5.949725 -6.120688
Si -2.341173 1.864637 -3.447246
Si -0.441401 3.317840 -5.315283
Si 1.897185 5.203643 -8.129377
Si -3.660943 3.326659 -8.683983
Si -1.209467 4.753400 -14.037298
Si 1.568833 7.357218 -11.696247
Si -0.679488 3.581375 -9.216847
Si -1.002470 5.694500 -11.177074
O 1.553480 6.820261 -7.966742
O 2.648957 4.565781 -6.799014
O 3.028723 4.958822 -9.306868
O -4.051362 2.393571 -7.367307
O -4.754993 4.486312 -9.045397

O -3.693335 2.193809 -9.914351
O 3.915470 2.115542 -6.972298
O 3.645988 -0.209122 -8.265114
O 2.788047 2.051098 -9.480638
O -2.821979 -0.556413 -9.479177
O -2.141853 -2.471785 -7.703764
O -3.425831 -0.249703 -6.821004
O -3.274697 5.170737 -6.221988
O -3.117050 2.521133 -2.141771
O -3.486377 1.402868 -4.538399
O -1.324761 0.663752 -2.945168
O 3.456417 1.992002 -4.145627
O 1.521650 2.143373 -2.336118
O 1.095172 0.515039 -4.396616
O -0.824448 -0.239687 -7.614295
O 1.464165 1.015674 -7.329197
O -0.400655 1.963065 -9.109098
O -0.799624 2.175950 -6.450729
O -1.458141 3.147716 -4.040916
O -0.591969 4.853402 -5.872374
O 1.142102 3.187761 -4.854358
O -3.968305 7.230939 -8.645881
O -1.492962 6.716387 -7.575505
O 0.500695 4.384770 -8.430185
O -2.128237 3.925782 -8.512180
O 0.969159 8.756828 -12.335895
O 2.774396 7.564736 -10.565865
O 2.267523 6.461585 -12.873922
O -2.315682 5.018819 -15.229794
O 0.339655 5.152191 -14.555458
O -1.368762 3.163576 -13.644381
O -1.463303 5.764930 -12.751142
O -0.742369 4.088374 -10.796192
O -2.213802 6.292374 -10.242551
O 0.353466 6.549608 -10.882309
N -1.997792 9.960602 -1.533376
N 0.339606 12.540091 -10.423355
C -2.055067 8.571737 -4.984804
C -2.135663 9.482632 -3.929293
C -1.968417 9.046080 -2.594210
C -1.706617 7.675642 -2.357925
C -1.625408 6.776632 -3.421213
C -4.224880 5.138765 -5.124430
C -1.799419 7.199942 -4.761780
C -1.894282 9.566935 -10.519746
C -1.252293 10.747160 -10.903484
C -0.279695 11.343279 -10.061313
C 0.008802 10.722695 -8.823163

C -0.642049 9.545376 -8.452616
 C -4.572920 8.047625 -7.611289
 C -1.603516 8.930820 -9.289380
 H 3.058650 2.991998 -9.533655
 H 3.049171 -0.948653 -8.064998
 H 3.654877 3.072353 -6.956517
 H 2.075787 4.286303 -6.048871
 H 0.585738 6.960393 -7.930198
 H 3.113965 5.702635 -9.945683
 H -3.720125 2.730922 -6.511861
 H -4.503939 5.418568 -8.848518
 H -4.133524 2.512801 -10.720204
 H -2.926427 -2.994652 -7.938927
 H -3.814498 0.607264 -7.128290
 H -3.116093 0.357331 -9.685515
 H -2.532687 10.806549 -1.710734
 H -2.222040 9.557704 -0.627163
 H -1.430450 5.724623 -3.199214
 H -1.563756 7.322372 -1.332347
 H -2.195436 8.945029 -6.001368
 H -2.325954 10.540958 -4.131815
 H -3.884385 4.450506 -4.337977
 H -4.362067 6.137388 -4.683874
 H -5.177435 4.781810 -5.538112
 H -3.888504 2.003476 -1.856043
 H -3.278179 0.660524 -5.154239
 H -0.617160 0.402031 -3.579903
 H 0.648897 1.788726 -2.079402
 H 3.743539 1.970093 -5.089390
 H 1.226249 0.331152 -5.348246
 H 0.369866 12.729650 -11.421564
 H 1.236395 12.715329 -9.977734
 H -0.379075 9.089149 -7.496084
 H 0.755358 11.166041 -8.158134
 H -2.616060 9.120603 -11.208598
 H -1.493972 11.215184 -11.861825
 H -4.215240 9.087653 -7.675285
 H -5.658831 8.031758 -7.771754
 H -4.348265 7.644105 -6.613828
 H 2.398570 7.731435 -9.674632
 H 0.339133 9.221571 -11.748557
 H 1.640072 6.084784 -13.529242
 H -1.085770 2.968376 -12.730380
 H 0.754092 4.455270 -15.094218
 H -2.112013 5.785364 -15.791608

The p-APTMS Monomer on Silica:
 Si O N C H

1.0000000000000000
 21.394899999999998 0.0000000000000000 0.0000000000000000
 0.0000000000000000 21.394899999999998 0.0000000000000000
 0.0000000000000000 0.0000000000000000 35.000000000000000
 Si O N C H
 103 232 1 8 63
 Direct
 0.9131395289548131 0.5250609614100358 0.0629610543365072
 0.4185063421126357 0.8406357774160044 0.0664938058056328
 0.7807030791472469 0.0655940550116815 0.0649382800419310
 0.6914261842108294 0.3937778489705456 0.0704579233936258
 0.0718846809523287 0.0115298336058892 0.0735949750655308
 0.2954207106488649 0.9187776206343288 0.0830699246474061
 0.6741597954208445 0.2536891731899479 0.0838596732914595
 0.1540108570798179 0.3236363751400828 0.0855087547963200
 0.9275801071183932 0.2764179207958734 0.0855495999795370
 0.1663469272576376 0.4739174521471777 0.0892993928408852
 0.2250073673133907 0.6720369626553871 0.0893651670381954
 0.6433913446920583 0.0323840076735946 0.0908568870833569
 0.1369816370762438 0.1384083753936136 0.0994376732956633
 0.3627090736013862 0.7291963530007489 0.1026215740639970
 0.3601550263984326 0.3881122323560806 0.1073889250038966
 0.0446281964189552 0.5535535855594578 0.1060600663243917
 0.0882521421158787 0.6978145128698141 0.1081936522624702
 0.6767705456415121 0.5773498855534284 0.1125863448645075
 0.5404500993109912 0.2667503210150357 0.1120675822788519
 0.4668337796033944 0.0114087470718597 0.1174394236892271
 0.7429332996401428 0.8681867341180940 0.1180565102966008
 0.5380072809245455 0.5303742321171914 0.1170620031051587
 0.3239785275443123 0.1455495826830386 0.1214055870317074
 0.8591898269241035 0.7741322086170013 0.1220390125060001
 0.0528010516035472 0.2468969460534625 0.1261196722147089
 0.4838144433771139 0.6678929533689006 0.1250105178435283
 0.8013483550833058 0.2544515670629515 0.1317494816896455
 0.8158886075536991 0.5224703821881587 0.1318385672888251
 0.2693708756579868 0.2818564294015163 0.1369041381830634
 0.4956351357110607 0.8752472978004731 0.1393856521312456
 0.2415293241547564 0.5557980334327506 0.1416527654621857
 0.4634438243772060 0.1462831738401579 0.1399550000097360
 0.8356614101874406 0.1128769254820591 0.1404792254090148
 0.3282387158040162 0.0069445073342631 0.1515421797862335
 0.0405056831402170 0.9517021184906778 0.1510877758051977
 0.7599532253869064 0.3939190319283739 0.1530188143725128
 0.5254568631903900 0.3968384330068528 0.1590524902734375
 0.6289146474221209 0.8179032057680841 0.1677018261593885
 0.8773901838875723 0.6501750865679223 0.1659022045454814
 0.3632364251485675 0.4943423350915440 0.1697507149574859
 0.7675250603845621 0.9918041386920234 0.1723442429719521

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0.3814639212019874 0.8133869624510985 0.1774554511908845
0.6379111789622340 0.0496983493318053 0.1813531050320001
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0.1560831788942411 0.9717551465669322 0.2009090857283697
0.0590303056604609 0.1838282226475206 0.2026724407648672
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0.6477544289520489 0.4252595940924920 0.2099541365995659
0.2882828528274361 0.9087162327962531 0.2114930349000652
0.1999309769468797 0.3327278343247232 0.2129920615133468
0.1780196704642202 0.5664072691963453 0.2208037907356662
0.4655754281378536 0.1765599493703446 0.2218902800907247
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0.4520658265829514 0.5679504166268885 0.2247656534432851
0.4616269497431468 0.3244200139034505 0.2227388198364817
0.7834824448298439 0.6839313396593852 0.2279735778336179
0.6040868517426499 0.5669774336568111 0.2309219065017358
0.0784842863810749 0.3939932330633836 0.2302484047262702
0.8625012237120113 0.9288711732199784 0.2309418060652178
0.2759083550479786 0.4541093795123423 0.2390802853165631
0.6022623519296406 0.3086989039974239 0.2490118757620833
0.6475109404225641 0.8609794551926514 0.2539730631736625
0.5811505644157849 0.9929847628694420 0.2527793245154468
0.2520571296819502 0.1158170951529200 0.2571112850426733
0.0797293492567967 0.6556044403501188 0.2571077748647112
0.9802222646881527 0.5535022076206039 0.2620985874392373
0.0313652620074396 0.2773859520214338 0.2698207490078200
0.9213772422159444 0.0403206184144154 0.2695456500886343
0.7855826083433113 0.8196112514791813 0.2693784819703952
0.5437540725198970 0.7599148290433916 0.2788804595280961
0.3523882895172227 0.3571959272368534 0.2825972387529470
0.1474379487703618 0.0140965999426485 0.2827171144951820
0.2385566842099192 0.2579432526834862 0.2835348264423769
0.3876466378787707 0.0993759486005432 0.2834697632418959
0.2888974663922301 0.8256279392392294 0.2883216933151828
0.6147091103690739 0.1208665267116709 0.2968407693610821
0.3753234862659178 0.5758610950928589 0.2996946639105408
0.4675179015640745 0.9796876230884121 0.3019454888774061
0.6348231509323127 0.6439342921890613 0.3078428168340027
0.7861831959330868 0.6408462218813106 0.3076654715083870
0.2947251320042714 0.6863838285747949 0.3091773088187239
0.1293794347138879 0.4531318924564506 0.3110798640476711
0.8804243627641249 0.5386322881439114 0.3146634621325411
0.0402394049066081 0.7697247566867114 0.3120123272892118

0.9093833790242125 0.2717142044276957 0.3183892250937697
0.1505655874760896 0.8728294155951951 0.3182366062930131
0.8505378061885411 0.1413349931566202 0.3198745994455920
0.5604040904090896 0.2428365855689154 0.3222764651845939
0.4307473999398147 0.8366413090221931 0.3228578273736203
0.2427988411961086 0.5566513972627234 0.3250517550808713
0.8846915634378169 0.7583339683243934 0.3224336029229465
0.9939474346247312 0.4779712833128559 0.3279410951972204
0.0328084120561691 0.0497262706715386 0.3292586222339534
0.1356747121157484 0.3119069428203693 0.3337356729324192
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0.7276088613072982 0.0943452645031962 0.3503464031475587
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0.4463714120724493 0.8552037394121688 0.0236755624784142
0.8879857653719191 0.5801384000763850 0.0338788904017314
0.7586979063490299 0.1165912838377213 0.0313578475936101
0.9275657816856719 0.4612454601811742 0.0378368758960457
0.1134200718862151 0.9787156311208243 0.0390600702659921
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The 2.0 p-APTMS/nm² Silica Model:

Si O N C H

1.0000000000000000

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0.0000000000000000 21.394899999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Si O N C H

111 248 9 72 151

Direct

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The 2.6 p-APTMS/nm² Silica Model:

Si O N C H

1.0000000000000000

21.394899999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.394899999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Si O N C H

114 254 12 96 184

Direct

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The 3.1 p-APTMS/nm² Silica Model:

Si O N C H

1.0000000000000000

21.394899999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.394899999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.000000000000000

Si O N C H

116 258 14 112 206

Direct

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The 3.3 p-APTMS/nm² Silica Model:

Si O N C H

1.0000000000000000

21.394899999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.394899999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Si O N C H

117 260 15 120 217

Direct

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The Clean Silica Surface:

Si O H

1.0000000000000000

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 0.0000000000000000 0.0000000000000000 35.0000000000000000

Si O H

102 230 52

Direct

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Methanol:

O C H

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0.0000000000000000 21.394899999999998 0.0000000000000000

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O C H

1 1 4

Direct

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p-APtMS Molecule:

Si O N C H

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0.0000000000000000 21.3948999999999998 0.0000000000000000

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Si O N C H

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Direct

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0.3898947565049942 0.2029505368558805 0.1476491179590907