Electronic Supplementary Information

Spontaneous S–Si bonding of alkanethiols to Si(111)–H: towards Si–molecule–Si circuits

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1. AFM characterization

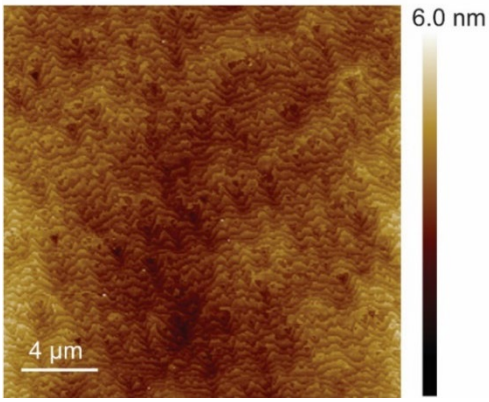


Figure S1. AFM characterisation of 20× 20 µm of a p–type Si(111)–H surface covered by dithiol **2**. The topography shows flat terraces separated by atomic steps. The peak-to-peak roughness measured within one Si(111) terrace is ca. 1.7 Å, consistent with an atomically smooth alkyl monolayer on Si(111). The high-quality topography confirms that the SAMs are homogeneous monolayers at the nanoscale, free of any contaminants or oxidative damage. AFM images of the same surfaces kept for 7 days under ambient condition did not show any sign of deterioration.

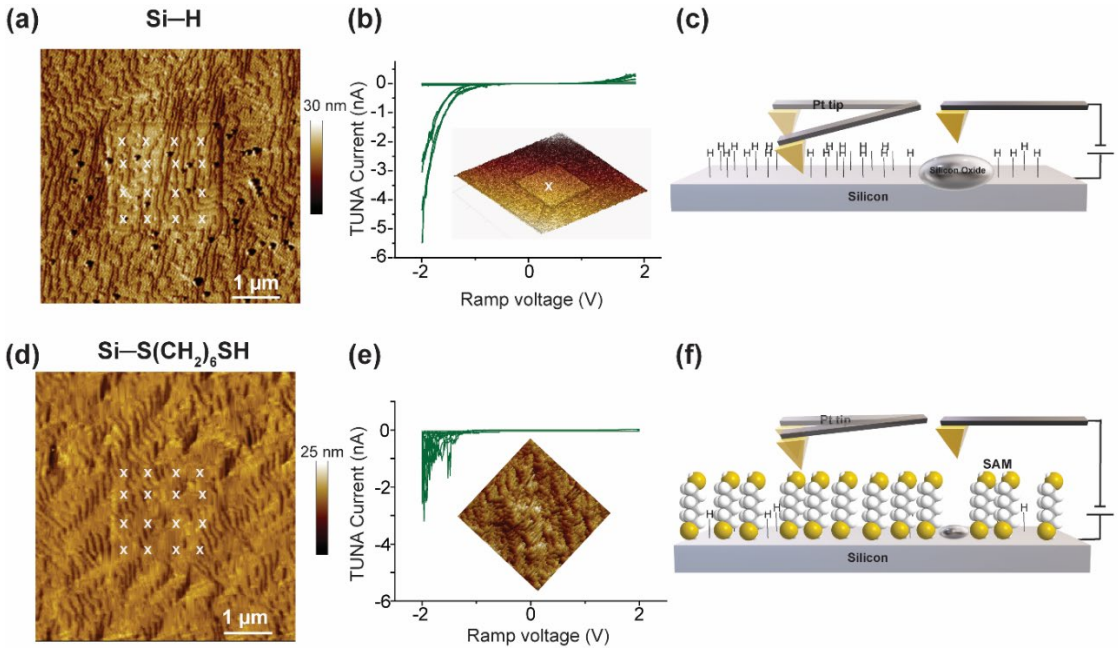


Figure S2. (a) and (d) show the topography images (5 × 5 µm) of the Si–H and the Si–$S(CH_2)_6SH$ after a squared (2 × 2) µm area in the center of the Si surface was held at +2 V for a period of 8 min with constant peak force of 554 nN . The "×" lables indicate the location where a bias sweep was applied. (b) and (e) show the current–volatge (I–V) sweeps applied on the bias-treated areas at the center of the surfaces. The I–V curves of the Si–$S(CH_2)_6SH$ surface are almost all rectifying (e) as expected for a platinum–n-type Si Shottky junction indicating that the hexanethiol monolayer prevent the surface from oxidation; however, after oxidation of the Si–H surface (b) a clearly AFM-visible oxide layer forms (3.0 ± 0.6 nm) which significantly blocks the current passing through the surface in more than 75% of the collected current–volatge curves meaning that the thin layer of oxide acts as dielectric film. Since the first step of oxidation of the Si surface requires the desorption of the –H or the –$S(CH_2)_6SH$, we conclude that the high density Si–$S(CH_2)_6SH$ monolayers are exceptional in preventing silicon oxidation. (c) and (f) are schematic diagrams of the studied surfaces.

2. X-ray Reflectometry (XRR)

Specular X-ray reflectometry at the solid-air interface was conducted on a Panalytical Ltd X′Pert Pro instrument with a rotating anode source (Cu Kα radiation, λ = 1.54 Å). The beam was focused using a Göbel mirror and collimated using fixed slits of 0.1 mm. The samples were mounted onto a motorised stage to adjust the sample into the optimal position for measurements. Angles of incidence were measured from 0.05° to 5.00° in 0.01° steps for 20 seconds per step. The raw data was reduced so that the critical edge was normalised to a reflectivity of unity and the data was presented as reflectivity versus momentum transfer, Q, defined as:

$$Q = \frac{4\pi \sin\theta}{\lambda}$$

where λ is the X-ray wavelength and θ is the angle of incidence. The data was analysed using MOTOFIT which utilises an Abele's matrix method. The monolayer was fitted using a single layer model with fitting parameters of thickness, roughness, and scattering length density (SLD), ρ, defined as:

$$\rho = \frac{r_e \sum Z_i}{V_m}$$

where V_m is the total molecular volume (determined to be 149 Å^3 for compound **2**), Z_i is the atomic number of each atom in the species, and r_e is the Bohr electron radius (2.818 ×10^{-5} Å). The theoretical SLD (ρ_t) of compound **2** was determined to be 15.6 ×10^{-6} Å^{-2}. The fitting parameters were varied using least-squares regression until the calculated reflectivity from the fit suitably matched the collected data. The number of molecules per cm^2 was determined from the fitted values as follows:

$$molecules\ per\ cm^2 = \frac{\tau \rho_f 10^{16}}{V_m \rho_t}$$

Where τ is the fitted thickness and ρ_f is the fitted SLD.

Table S1. Theoretical parameters used in the modelling.

Molecule	Calculated SLD / ×10^{-6} Å^{-2}	Estimated maximum thickness / Å	Estimated volume / Å^3
1,6-hexandithiol	15.6	11.3	149

Table S2. Fitted SAM thickness and surface roughness (in Å), and fitted SLD (in 10^{-6} Å^{-2}) for **2** on Si(111)–H as determined from XRR data (see XRR curves in Fig. 2c).

Monolayer	Thickness / Å	Fitted SLD / ×10^{-6} Å^{-2}	Volume fraction	Molecules per cm^2	coverage %	Roughness of Si-monolayer interface/ Å	Roughness of monolayer-air interface / Å
Low doped n	9.1 ± 0.2	13.7 ± 0.2	0.878 ± 0.013	5.36 ×10^{14}	68	0.6 ± 0.1	4.4 ± 0.1
Low doped p	10.4 ± 0.5	13.8 ± 0.2	0.885 ± 0.012	6.17 ×10^{14}	78	1.1 ± 0.2	4.6 ± 0.1
High doped n	8.5 ± 0.6	15.3 ± 0.1	0.981 ± 0.006	5.59 ×10^{14}	71	3.9 ± 0.1	13.3 ± 0.3
High doped p	11.1 ± 0.4	13.9 ± 0.3	0.891 ± 0.019	6.64 ×10^{14}	84	2.9 ± 0.1	7.3 ± 0.2

The SLD of air and silicon was fixed to 0 and 20.1 ×10^{-6} Å^{-2} respectively.

3. Initiation and then propagation of a free-radical polymerization process

This section provides more details of the initiation and propagation reactions depicted in Figure 4, involving the model compound RSH (R = C_3H_7) reacting with Si(111)–H.

Figure 4 shows a reaction scheme involving initiation of the surface reaction and then propagation of a free-radical polymerization process at low coverage, showing calculated Gibbs free energies. The corresponding figure showing the purely electronic energy differences is Figure S3.

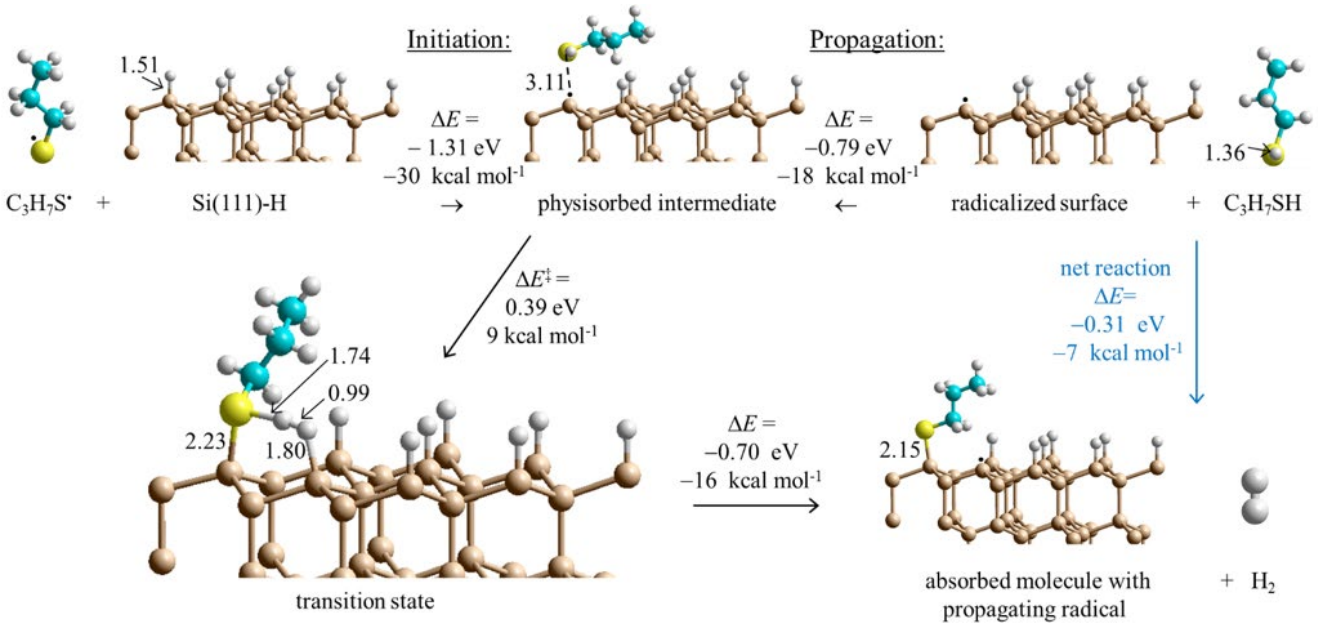


Figure S3. DFT mechanism for SAM formation starting at low coverage. Calculations indicate that thiyl radicals (RS•, with here R = C_3H_7) produced by attack of solution O_2 on the thiol reactants (RSH) react with Si(111)–H to abstract hydrogen and for thiol physisorbed to a silicon surface radical (black dot). Reaction over a barrier then leads to chemisorption and radical regeneration. This provides initiation for a free-radical polymerization reaction that then covers the surface with adsorbate. Some critical bond lengths are shown, in Å; only one copy of the used 3×3 supercell is shown. These results show the electronic energy changes coming from the VASP calculations that are analogous to the Gibbs free energy changes shown in Figure 4.

The transition state shown in these figures is a very complex one involving simultaneous motion involving changes to the Si–S, S–H, H–H, and Si–H bond lengths: the reaction involves the near-synchronous breaking of two bonds and reformation of another two. Initial calculations were performed on a model compound, freezing the coordinates of the external silicon atoms to coincide with locations on the 2D Si(111)–H surface. This cluster, as well as the energetics analogous to those shown in Figure S4, are provided in Figure S3. The results are quite similar to those subsequently optimized for the 2D surface. Indeed, the optimization of the transition structure for the 2D materials was made starting at the results for the model compound.

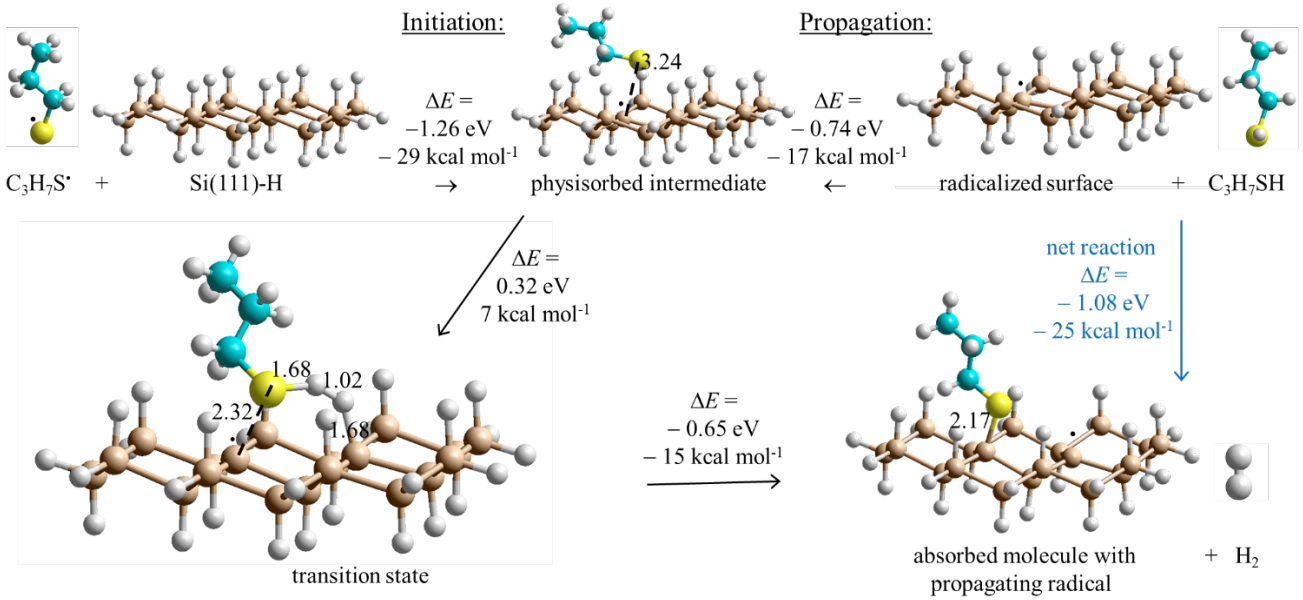


Figure S4. DFT mechanism for SAM formation based on the properties of a model compound. Calculations indicate that thiyl radicals (RS•, with here R = C_3H_7) produced by attack of solution O_2 on the thiol reactants (RSH) react with Si(111)–H to abstract hydrogen and for thiol physisorbed to a silicon surface radical (black dot). Reaction over a barrier then leads to chemisorption and radical regeneration. This provides initiation for a free-radical polymerization reaction that then covers the surface with adsorbate. Some critical bond lengths are shown, in Å.

There is one significant difference found between the results for the model compound and the 2D surface: a second intermediary species was found for the 2D surface, displaying a chemisorbed thiol with in which sulfur forms three covalent bonds. It is only a shallow minimum on the potential-energy surface and hence was not depicted in the primary results in Figure 4. Its structure and properties are given in Figure S4.

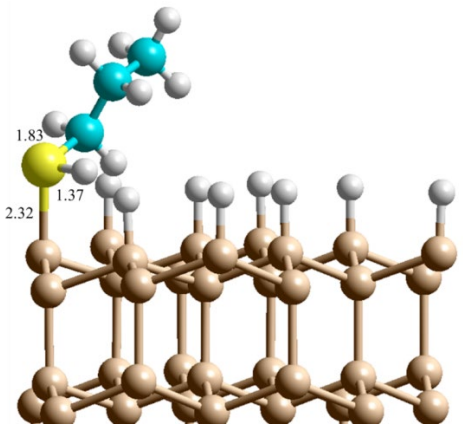


Figure S5. A chemisorbed intermediate found on the 2D surface, showing the covalent-bond lengths to sulfur, in Å.

Notwithstanding this difference, the reaction profiles for the model cluster and 2D surface are similar. The energy profiles and key coordinate changes as a function of an internal reaction coordinate (defines as the integral of the accumulated bond-length changes in the 4 key bonds) are shown in Figure S6. The Si–S and H–H bonds are largely formed at the transition state whilst the Si–H and S–H bonds are just beginning to break. On the 2D surface, the transition state occurs slightly later than it does for the model cluster.

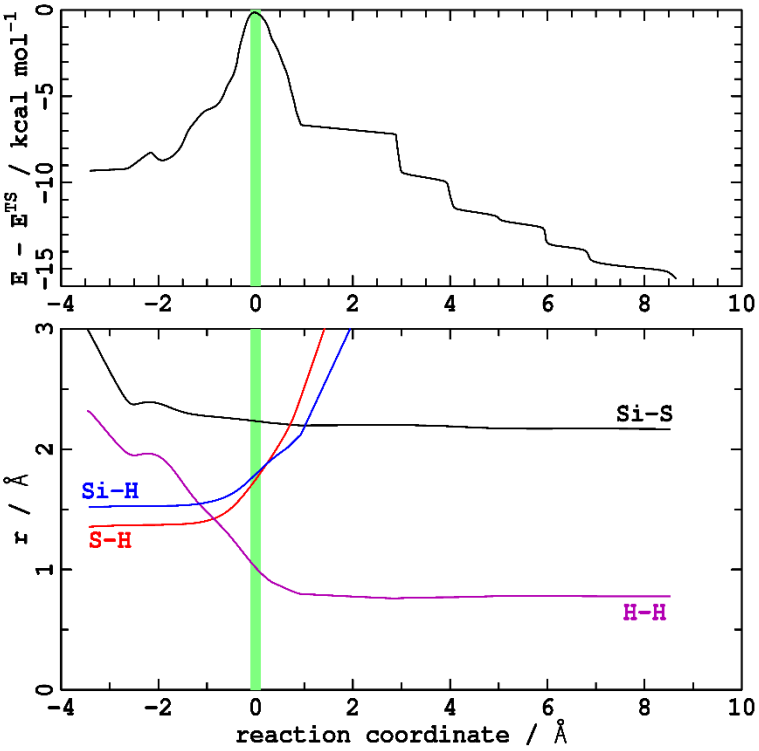


Figure S6. The top frame shows the energy calculated for the indicated model cluster system as a function of a continuous reaction coordinate, going from the physisorbed intermediate over the transition state to form products. The lower frame shows the critical Si–S, S–H, H–H, and H–Si bond lengths (see Figure 4) along this reaction coordinate. While at the transition state, the H–H and Si–S bonds are largely formed whilst the S–H and Si–H are largely unbroken, critical changes to all 4 bond lengths do occur at this structure. The reaction coordinate follows the eigenvector of the hessian matrix with imaginary eigenvalue away from the transition state (green region), but afterwards becomes the results of unconstrained geometry optimization. The reaction profile for the model compound is similar.

4. SAM completion at high coverage for the binding of 2 to Si(111)–H

Calculations on a 3×3 supercell for the binding of **2** to Si(111)–H at high coverage are reported. In this lattice, the chemical state of the 9 surface silicon atoms can be represented by the formula

$$(\mathrm{SiH})_i\mathrm{Si}^{\bullet}_j(\mathrm{SiSR})_k \quad \text{where } i+j+k=9$$

and R = $S(CH_2)_6SH$. At the low coverage of 1:9, the structure of $(\mathrm{SiH})_8\mathrm{Si}^{\bullet}_0(\mathrm{SiSR})_1$, shown in Figure 5a, has the alkane chains oriented at an angle of 70° to the surface. On this surface, initiation occurs through the reaction (akin to Figure 5)

$$(\mathrm{SiH})_9\mathrm{Si}^{\bullet}_0(\mathrm{SiSR})_0 + \mathrm{RS}^{\bullet} \rightarrow (\mathrm{SiH})_8\mathrm{Si}^{\bullet}_1(\mathrm{SiSR})_1 + \mathrm{H}_2$$

followed by the free-radical polymerization reaction

$$(\mathrm{SiH})_{9-n}\mathrm{Si}^{\bullet}_1(\mathrm{SiSR})_{n-1} + \mathrm{RSH} \rightarrow (\mathrm{SiH})_{9-n-1}\mathrm{Si}^{\bullet}_1(\mathrm{SiSR})_n + \mathrm{H}_2$$

which can, in principle, occur for n = 2 to 8, the final product being the isolated surface radical $(SiH)_0Si_1^{\bullet}(SiSR)_8$. Figure 5b shows the species with n = 7 that forms part of this sequence, $(SiH)_1Si_1^{\bullet}(SiSR)_7$. DFT predicts the reaction leading to its production

$$(SiH)_2Si_1^{\bullet}(SiSR)_6 + RSH \rightarrow (SiH)_1Si_1^{\bullet}(SiSR)_7 + H_2$$

to be exothermic, with ΔE = -15 kcal mol^{-1}. However, as Frame c in Figure 5 shows, in this structure six chairs are forces to align vertically whilst one slightly lays over, taking on an orientationally partially disordered structure in which the 7 chains quickly adjust be become roughly equally spaced. The inter-chain separation is ca. 4.3 Å, close to the optimal distances found in 3D alkane materials and in monolayers on surfaces. Adding more ligands to this structure therefore requires compression of the ligands, with effectively all of the compression energy of all of the ligands needed to be costed during the next step in the polymerization process. As a result, the calculated reaction energy for the next step,

$$(SiH)_1Si_1^{\bullet}(SiSR)_7 + RSH \rightarrow (SiH)_0Si_1^{\bullet}(SiSR)_8 + H_2$$

is predicted to be endothermic, with ΔE = +44 kcal mol^{-1}. The free-radical polymerization mechanism therefore cannot proceed beyond a coverage of 7:9.

Also, free-radical polymerization can only proceed if the silicon free radical $Si^{\bullet}$ is located on an adjacent site to a SiH bond. During SAM polymerization, several Si–H bonds could be located adjacent to $Si^{\bullet}$, meaning that the path that the polymerization takes across the 2D surface is not controlled. Hence it is possible to produce silicon radicals that are not adjacent to Si–H, prematurely terminating chain propagation. Similarly, the SAM may grow in ways that leave one or more Si–H bonds surrounded by SiSR and hence unavailable for a chain-propagation reaction. It is therefore likely that the chain propagation reaction will lead to a SAM containing many defects.

If the SAM is in thermodynamic equilibrium, then such defects would be healed by annealing. Even in SAMs held together only by van der Waals forces, thermodynamic equilibrium is difficult to establish, making final compositions controlled by kinetic rather than thermodynamic factors. However, key steps in the formation process may be under thermodynamic control, and these can manifest to control some key final outcomes. In this case, calculations indicate that the transition state for the addition of the eighth ligand above remains accessible from the intermediate state (by analogy to Figure 5c), it is just that the precursor state itself becomes energetically unattainable. Understanding SAM properties then comes down to understanding the energetics of reactions that would anneal the SAM.

We have considered two processes for the model compound with R = C_3H_7, a species for which annealing reactions would be thought to be easier than for **2**. First, we examined the interchange of the ligand from an SiSR site to a neighbouring $Si^{\bullet}$ site. Accurate transition-state energies were not obtained, but many possible paths were examined with estimated barriers in the 40-50 kcal mol^{-1} range. To anneal SAMs at room temperature within 24 hours, barriers of at most 25 kcal mol^{-1} could be envisaged. Second, we considered processes in which the ligand on an SiSR site interchanges with the hydrogen on a neighbouring Si–H site, possible through a self-catalysed thiol intermediate. Again, no pathway under 40 kcal mol^{-1} could be envisaged. These results suggest that produced SAMs are kinetically trapped post production.

If the reactions are performed in solutions containing molecular oxygen and thiols, then small amount of thiyls present in solution could continue to react with partially formed SAMs. Of most significance, the most difficult reaction to complete, the reaction of a radical SAM at 8:9 coverage to form a SAM at 1:1 coverage, i.e.

$$(SiH)_0Si_1^{\bullet}(SiSR)_8 + RS^{\bullet} \rightarrow (SiH)_0Si_0^{\bullet}(SiSR)_9$$

is predicted to be exothermic, with ΔE = -45 kcal mol^{-1} for R = $(CH_2)_6SH$. The energy released by the fusing of the two radicals to form a Si–S bond is sufficient to compress the SAM into the extremely tight structure shown in Fig. 4c. If that silicon surface radical can react with solution radicals, then so can any other similar species have produced during the SAM formation process.

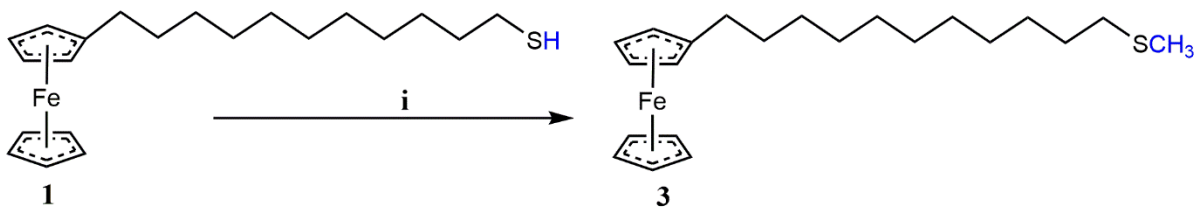
Next, we consider the reaction of an isolated SiH group with an RS$^{\bullet}$ radical from solution. The hydrogen abstraction reaction

$$(SiH)_1Si_0^{\bullet}(SiSR)_8 + RS^{\bullet} \rightarrow (SiH)_0Si_1^{\bullet}(SiSR)_8 + RSH$$

is predicted to be exothermic, with ΔE = -12 kcal mol^{-1}. This reaction introduces no new compression to the SAM and gains its exothermicity from the difference in S–H and Si–H bond strengths. After it is completed, a silicon surface radical is produced that can then react with a second thiyl from solution to complete the SAM.

The difficulty in doing these reactions, controlling their transition-state energies, will be the compression of the SAM that must be introduced prior to the meeting of the reacting atoms. These barriers will be strongly ligand-size dependent, suggesting that an optimum chain length will exist for producing regular SAMs. They will also strongly depend on the precise chemical structure of the defect being attacked by the radical. Basically, reactions on defects in SAMs at below 7:9 coverage will be expected to proceed based only on the availability of surface radicals, whereas reactions involving species at 1:1 coverage will experience high barriers. These high barriers may well exceed 25 kcal mol^{-1} and hence prevent SAMs forming at these coverages.

5. Synthesis of 11-(ferrocenyl)undecyl methyl sulphide (3)



Scheme 1. Synthesis of compound **3**

Reagents: 9) MeOH, DMF, NaOH, CH_3I, 0 ºC, 10 min.

All chemicals used for the synthesis of 11-(ferrocenyl)undecyl methyl sulphide **(3)** were of analytical grade and used as received. 11-(Ferrocenyl)undecanethiol (**(1)**, 95.0%), iodomethane (99.0%), methanol (97.0%), deuterochloroform (99.8%), N,N-dimethylformamide (99.8%), chloroform (98.0%) and hexane (98.0%) were purchased from Sigma-Aldrich and sodium hydroxide (97.0%) was purchased from Ajax fine chem. Milli-Q water (>18 MΩ cm) was used for cleaning and the preparation of solutions. The synthesis of **3** is based on a procedure reported by Yasuhiro. M et al.(Ann. Nucl. Med. 1993, 7, 173-177). Briefly, to a solution **2** (74.4 mg, 0.1 mmol) in 10 mL of MeOH: DMF (1:1) was added 10 mL of NaOH (1 M). Iodomethane (0.11 mmol, 13.68 µL) was cooled down to 0 ºC and added to the mixture with continuous stirring for 10 min at 0 ºC (Scheme 1). The organic phase was then extracted using chloroform, evaporated and purified by gradient column chromatography using hexane. The purified form of **3** is then dried under vacuum resulting in a pale-yellow solid (46.4 mg, 60% yield). ^{1}H NMR 400 MHz (CDCl3): δ (ppm) = 4.08 (s, 5H), 4.02 (s, 4H), 2.47 (m, 2H), 2.30 (t, 2H), 2.11 (s, 3H) for the added methyl group, 1.55 (m, 4H), 1.47 (m, 2H), 1.36 (m, 2H), 1.28 (m, 10H). ^{13}C{1H} NMR (101 MHz, CDCl3): δ (ppm) = 15.61 (CH_3), 28.85 (CH_2), 29.21 (CH_2), 29.27 (CH_2), 29.54 (CH_2), 29.61 (CH_2), 29.67 (CH_2), 31.14 (CH_2), 34.38 (CH_2), 53.41 (CH_2, next to ferrocene ring), 67.05 (CH), 68.14 (CH), and 68.50 (CH). HRMS (ESI) m/z calculated for **3** [M+H]+ 386.1725, found 386.1720.

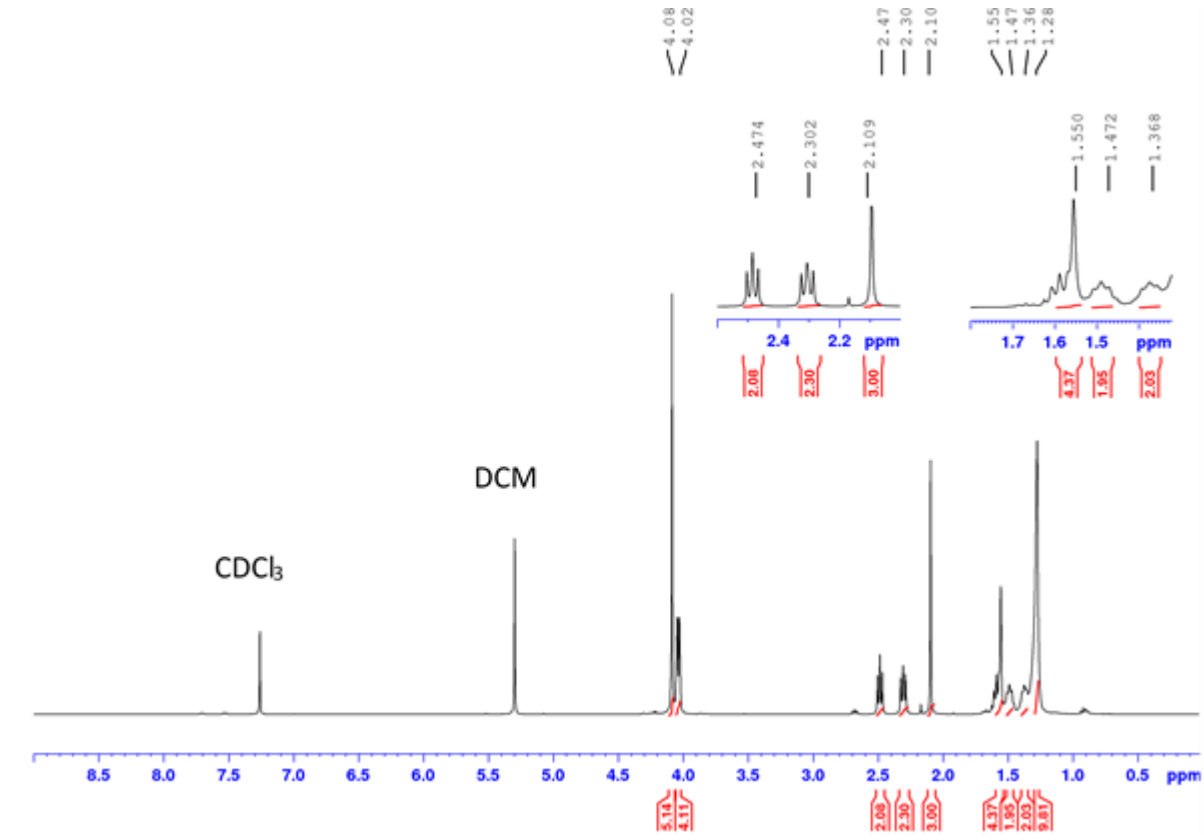


Figure S7. ^{1}H NMR 400 MHz ($CDCl_3$) spectrum of **3**

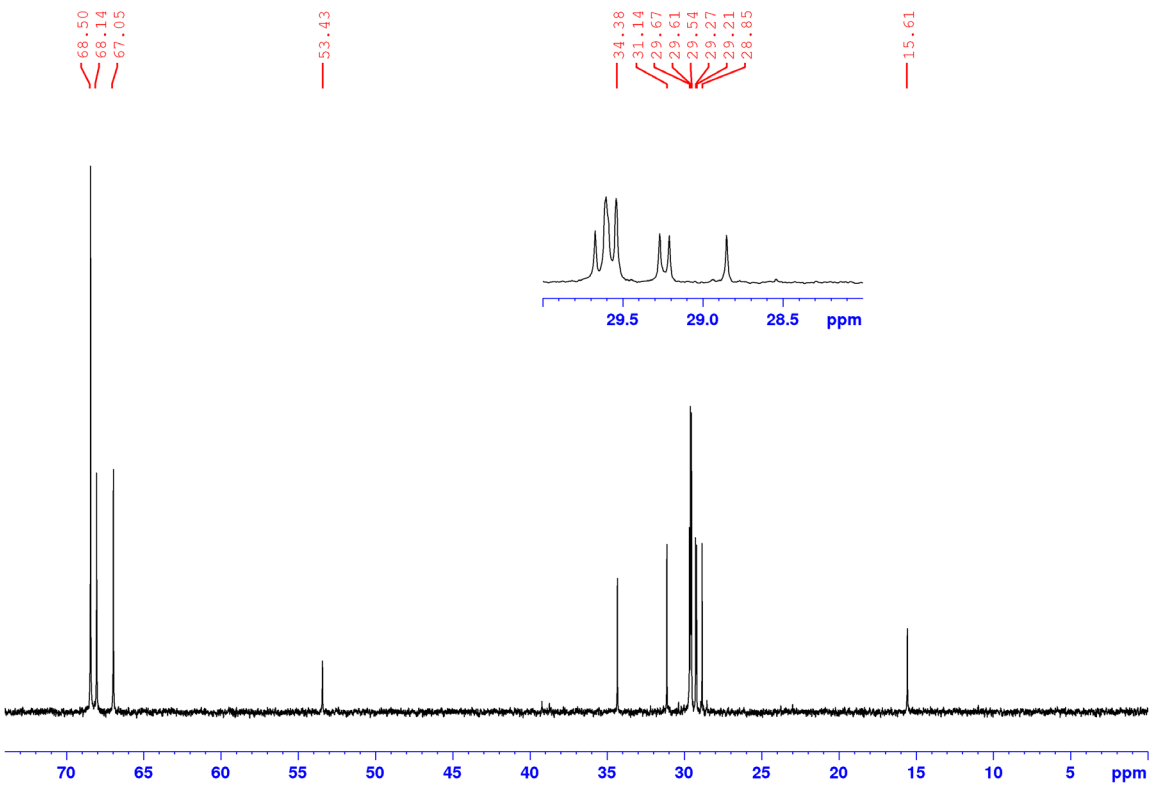


Figure S8. ^{13}C NMR ($CDCl_3$, 101 MHz) spectrum of **3**

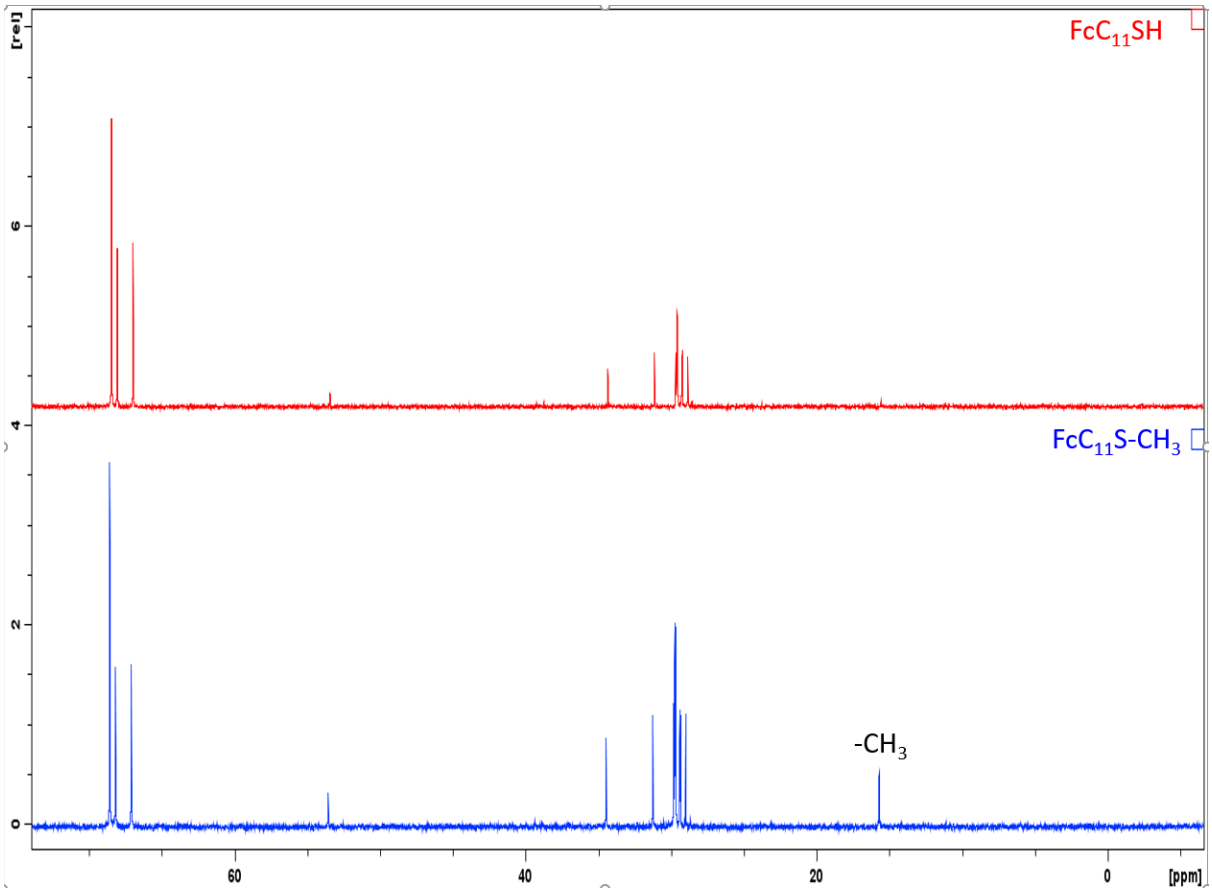


Figure S9. ^{13}C NMR spectra for **3** (blue) and **2** (red) with the methyl signal in **3** at δ=15.7.

6. XPS analysis of 3

The XPS spectra of Si(111)−H, incubated in 4 mM DCM solution of **3** for 24 h did not show evidence of S−Si emission at 162 eV. The observed shoulder between 162 and 164 eV is ascribed to Si plasmon loss which is also present in untreated Si(111)−H (Figure S11). Further, high resolution XPS data of the Si 2p envelope showed in addition to an emission centred at 99.5 eV assigned to the Si−Si bonding, a weak emission at 103 eV assigned to SiOx. The presence of a silica-related band suggests that the Si(111)−H surface is prone to oxidation in the absence of a monolayer. This indicates that **3** does not form a monolayer.

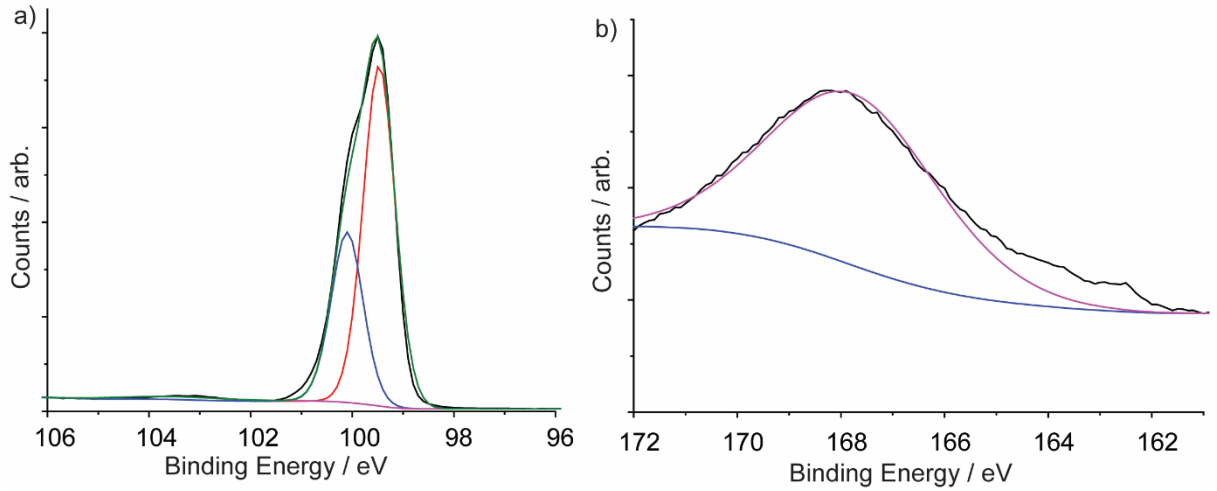


Figure S10. a) XPS High-resolution Si 2p emission and b) S 2p emission for a Si(111)−H surface incubated in 4 mM DCM solution of **3** for 24 h.

As a control measurement on the background signal of the Si electrode surface, we performed an XPS measurement for a freshly etched, unmodified Si(111)−H electrode (see Figure S11 below). Si 2p emission showed a background emission alongside the high intensity Si plasmon loss peak at 168 eV.

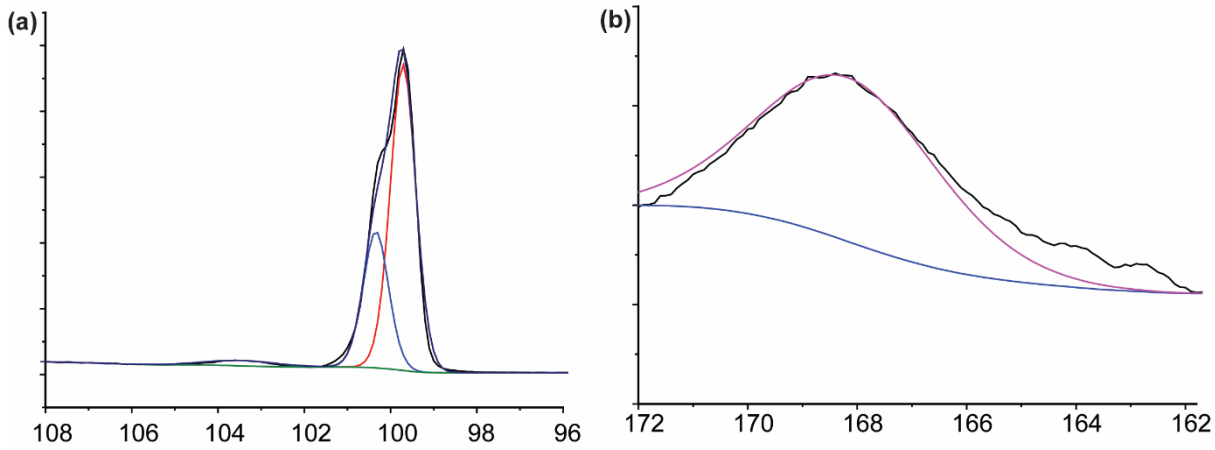


Figure S11. a) XPS high resolution Si 2p emission and b) S 2p emission for untreated Si(111)−H electrode stored in DCM for 24 h.

7. Electrochemical characterisation of 3

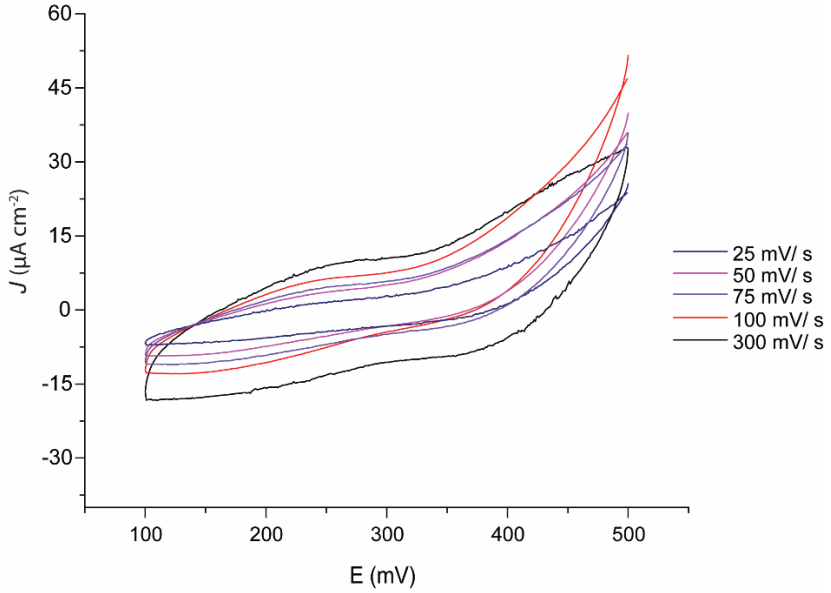


Figure S12. Cyclic voltammograms of Si(111)−H surface incubated in 4 mM DCM solution of **3** for 24 h. The voltammograms show absence of ferrocene signals and an increase in current beyond + 400 mV, indicating surface oxidation in the absence of a monolayer, suggesting that **3** does not form a monolayer on Si(111)–H surfaces.

8. STMBJ plateau length and blinking duration histograms

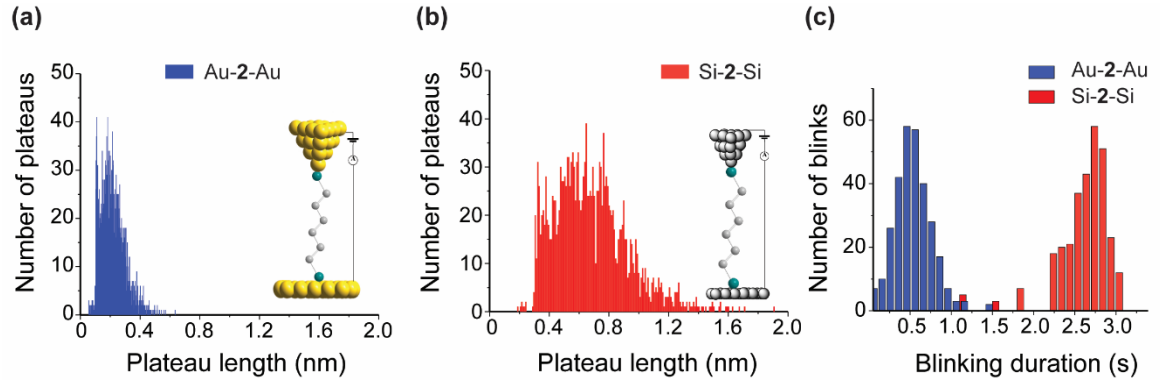


Figure S13. (a) Plateau length histogram for Au–**2**–Au with average plateau length of 0.25 nm (b) Plateau length histogram of Si–**2**–Si junctions with average plateau length of 0.70 nm. This suggests that due to the enhanced mechanical stability, the Si–**2**–Si junctions are resistant to breakage during the entire pulling cycle while the typical Au–**2**–Au junctions break before a full molecular stretch. (c) Blinking duration histograms when **2** is bonded to two Au electrodes (blue) versus when bonded to two Si electrodes (red) with average lifetime of 0.56 s and 2.70 s, respectively.

9. DFT optimized coordinates for all optimized 2D structures and associated molecules.

Table of Contents:

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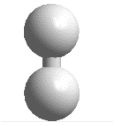
1. H2



E= -6.7341 eV, Ggas= -6.7704 eV, Gsoln= -6.6905 eV
box: 20.000000 0 0 0 20.000000 0 0 0 20.000000
Kpoints: 1 1 1
basis: NGX= 120 NGY= 120 NGZ= 120 NGXF= 180 NGYF= 180 NGZF= 180
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1	0.000000	0.000000	0.375100

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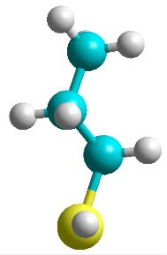
2. C3H7SH



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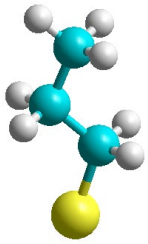
box: 25.000000 0 0 0 25.000000 0 0 0 25.000000
Kpoints: 1 1 1
basis: NGX= 192 NGY= 192 NGZ= 192 NGXF= 280 NGYF= 280 NGZF= 280
Low Frequencies (cm^-1)= 113. 207. 221. 248. 356. 689.

16	5.774760	3.958660	3.929870
6	1.578410	4.072160	4.007270
6	2.991270	3.492330	3.929180
6	4.063410	4.566480	4.082810
1	1.408350	4.583690	4.967520
1	0.819210	3.282340	3.911090
1	1.402680	4.804700	3.204090
1	3.129040	2.733510	4.717890
1	3.140860	2.970610	2.970600
1	3.951590	5.103470	5.037250
1	3.975140	5.316540	3.280420
1	5.728320	3.096880	4.969450

---

3. C3H7S

E= -55.9896 eV, Ggas= -54.3086 eV, Gsoln= -54.2287 eV
box: 25.000000 0 0 0 25.000000 0 0 0 25.000000
Kpoints: 1 1 1
basis: NGX= 192 NGY= 192 NGZ= 192 NGXF= 280 NGYF= 280 NGZF= 280
Low Frequencies (cm^-1)= 114. 224. 226. 357. 477. 724.

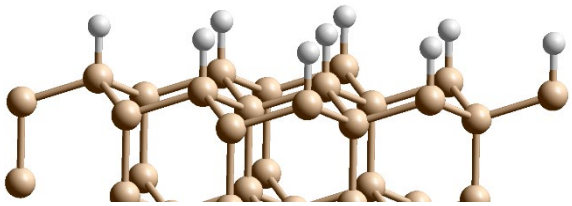


16 5.763980 3.981500 3.960160
6 1.579950 4.072510 4.007240
6 2.988330 3.483920 3.926860
6 4.070660 4.554140 4.061620
1 1.411880 4.583810 4.968070
1 0.816290 3.287340 3.910580
1 1.406070 4.806390 3.204560
1 3.134310 2.730300 4.716850
1 3.128180 2.958110 2.969160
1 3.977130 5.097910 5.021530
1 3.954570 5.336900 3.287330

---

4. Si(111)-H 3x3

E= -468.8368 eV, Ggas= -463.5937 eV, Gsoln= -463.5138 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 70 NGY= 70 NGZ= 180 NGXF= 100 NGYF= 100 NGZF= 270
Low Frequencies (cm^-1)= 44. 44. 77. 77. 77. 77.



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14 6.440293 3.861800 2.000000
14 10.267155 3.861800 2.000000
14 4.526862 7.175959 2.000000
14 8.353724 7.175959 2.000000
14 12.180586 7.175959 2.000000
14 0.700000 0.547640 2.000000
14 4.526862 0.547640 2.000000
14 8.353724 0.547640 2.000000
14 10.267155 1.652360 2.781155
14 2.613431 1.652360 2.781155
14 6.440293 1.652360 2.781155
14 12.180586 4.966520 2.781155
14 4.526862 4.966520 2.781155
14 8.353724 4.966520 2.781155
14 14.094017 8.280679 2.781155
14 6.440293 8.280679 2.781155
14 10.267155 8.280679 2.781155
14 10.267155 1.652360 5.124620
14 2.613431 1.652360 5.124620
14 6.440293 1.652360 5.124620
14 12.180586 4.966520 5.124620
14 4.526862 4.966520 5.124620
14 8.353724 4.966520 5.124620
14 14.094017 8.280679 5.124620
14 6.440293 8.280679 5.124620
14 10.267155 8.280679 5.124620
14 12.180586 2.757080 5.905775
14 4.526862 2.757080 5.905775
14 8.353724 2.757080 5.905775
14 14.094017 6.071239 5.905775
14 6.440293 6.071239 5.905775
14 10.267155 6.071239 5.905775
14 16.007448 9.385399 5.905775
14 8.353724 9.385399 5.905775
14 12.180586 9.385399 5.905775
14 12.180586 2.757080 8.249553
14 4.526862 2.757080 8.249553
14 8.353724 2.757080 8.249553
14 14.094017 6.071239 8.249553
14 6.440293 6.071239 8.249553
14 10.267155 6.071239 8.249553
14 16.007448 9.385399 8.249553

14 8.353724 9.385399 8.249553
14 12.180586 9.385399 8.249553
14 2.613431 3.861800 9.033240
14 6.440293 3.861800 9.033240
14 10.267155 3.861800 9.033240
14 4.526862 7.175959 9.033240
14 8.353724 7.175959 9.033240
14 12.180586 7.175959 9.033240
14 0.700000 0.547640 9.033240
14 4.526862 0.547640 9.033240
14 8.353724 0.547640 9.033240
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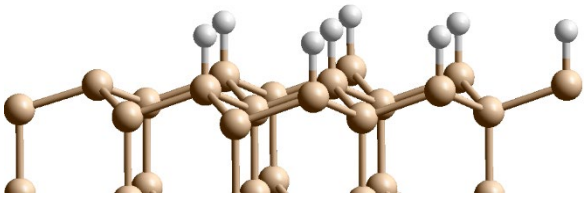
14 6.440293 3.861800 11.378206
14 10.267155 3.861800 11.378206
14 4.526862 7.175959 11.378206
14 8.353724 7.175959 11.378206
14 12.180586 7.175959 11.378206
14 0.700000 0.547640 11.378206
14 4.526862 0.547640 11.378206
14 8.353724 0.547640 11.378206
14 10.267155 1.652360 12.145176
14 2.613431 1.652360 12.145176
14 6.440293 1.652360 12.145176
14 12.180586 4.966520 12.145176
14 4.526862 4.966520 12.145176
14 8.353724 4.966520 12.145176
14 14.094017 8.280679 12.145176
14 6.440293 8.280679 12.145176
14 10.267155 8.280679 12.145176
1 2.613431 3.861800 0.495623
1 6.440293 3.861800 0.495623
1 10.267155 3.861800 0.495623
1 4.526862 7.175959 0.495623
1 8.353724 7.175959 0.495623
1 12.180586 7.175959 0.495623
1 0.700000 0.547640 0.495623
1 4.526862 0.547640 0.495623
1 8.353724 0.547640 0.495623
1 10.267155 1.652360 13.650245
1 2.613431 1.652360 13.650245
1 6.440293 1.652360 13.650245
1 12.180586 4.966520 13.650245
1 4.526862 4.966520 13.650245
1 8.353724 4.966520 13.650245
1 14.094017 8.280679 13.650245
1 6.440293 8.280679 13.650245
1 10.267155 8.280679 13.650245

---

5. Si(111)-H 3x3 radical, with one removed H

E= -464.3662 eV, Ggas= -459.2202 eV, Gsoln= -459.1403 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 70 NGY= 70 NGZ= 180 NGXF= 100 NGYF= 100 NGZF= 270
Low Frequencies (cm^-1)= 53. 53. 76. 76. 85. 85.



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14 6.440293 3.861800 2.000000
14 10.267155 3.861800 2.000000
14 4.526862 7.175959 2.000000
14 8.353724 7.175959 2.000000
14 12.180586 7.175959 2.000000
14 0.700000 0.547640 2.000000
14 4.526862 0.547640 2.000000
14 8.353724 0.547640 2.000000
14 10.267155 1.652360 2.781155
14 2.613431 1.652360 2.781155
14 6.440293 1.652360 2.781155
14 12.180586 4.966520 2.781155

14	4.526862	4.966520	2.781155
14	8.353724	4.966520	2.781155
14	14.094017	8.280679	2.781155
14	6.440293	8.280679	2.781155
14	10.267155	8.280679	2.781155
14	10.267155	1.652360	5.124620
14	2.613431	1.652360	5.124620
14	6.440293	1.652360	5.124620
14	12.180586	4.966520	5.124620
14	4.526862	4.966520	5.124620
14	8.353724	4.966520	5.124620
14	14.094017	8.280679	5.124620
14	6.440293	8.280679	5.124620
14	10.267155	8.280679	5.124620
14	12.180586	2.757080	5.905775
14	4.526862	2.757080	5.905775
14	8.353724	2.757080	5.905775
14	14.094017	6.071239	5.905775
14	6.440293	6.071239	5.905775
14	10.267155	6.071239	5.905775
14	16.007448	9.385399	5.905775
14	8.353724	9.385399	5.905775
14	12.180586	9.385399	5.905775
14	12.181217	2.756716	8.254655
14	4.526231	2.756716	8.254655
14	8.353724	2.757175	8.251226
14	14.094017	6.073097	8.248484
14	6.440375	6.071192	8.251226
14	10.267073	6.071192	8.251226
14	16.005839	9.384470	8.248484
14	8.353724	9.386128	8.254655
14	12.182195	9.384470	8.248484
14	2.613431	3.863995	9.034570
14	6.440675	3.862020	9.036921
14	10.266773	3.862020	9.036921
14	4.526760	7.176018	9.033783
14	8.353724	7.175518	9.036921
14	12.180688	7.176018	9.033783
14	0.698099	0.546543	9.034570
14	4.528763	0.546543	9.034570
14	8.353724	0.547522	9.033783
14	2.613431	3.866698	11.386741
14	6.440742	3.862059	11.382304
14	10.266706	3.862059	11.382304
14	4.527466	7.175610	11.378639
14	8.353724	7.175441	11.382304
14	12.179982	7.175610	11.378639
14	0.695758	0.545191	11.386741
14	4.531104	0.545191	11.386741
14	8.353724	0.548337	11.378639
14	10.264803	1.653773	12.150988
14	2.613431	1.652360	12.080753
14	6.442645	1.653773	12.150988
14	12.178186	4.967851	12.150988
14	4.529262	4.967851	12.150988
14	8.353724	4.966520	12.148100
14	14.094017	8.280679	12.142359
14	6.440341	8.277935	12.150988
14	10.267107	8.277935	12.150988
1	2.613431	3.861401	0.495677
1	6.440134	3.861708	0.495643
1	10.267314	3.861708	0.495643
1	4.527850	7.175389	0.495642
1	8.353724	7.176142	0.495643
1	12.179598	7.175389	0.495642
1	0.700345	0.547839	0.495677
1	4.526517	0.547839	0.495677
1	8.353724	0.548781	0.495642
1	10.262957	1.652800	13.655456
1	6.444491	1.652800	13.655456
1	12.178106	4.969936	13.655456

1 4.529342 4.969936 13.655456
1 8.353724 4.966520 13.652730
1 14.094017 8.280679 13.647456
1 6.438575 8.276824 13.655456
1 10.268873 8.276824 13.655456

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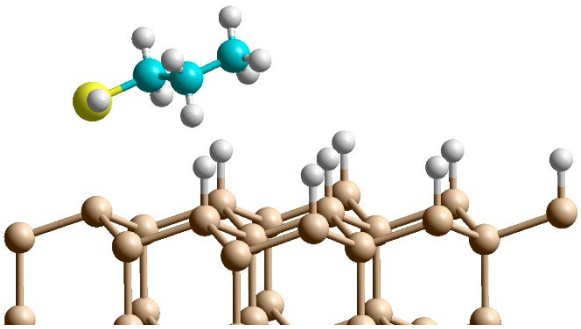
6. Si(111)-H 3x3 radical, physisorbed intermediate with C3H7SH

E= -526.1381 eV, Ggas= -518.5026 eV, Gsoln= -518.4227 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 224 NGXF= 126 NGYF= 126 NGZF= 336
Low Frequencies (cm^-1)= -44. 15. 36. 47. 53. 54.



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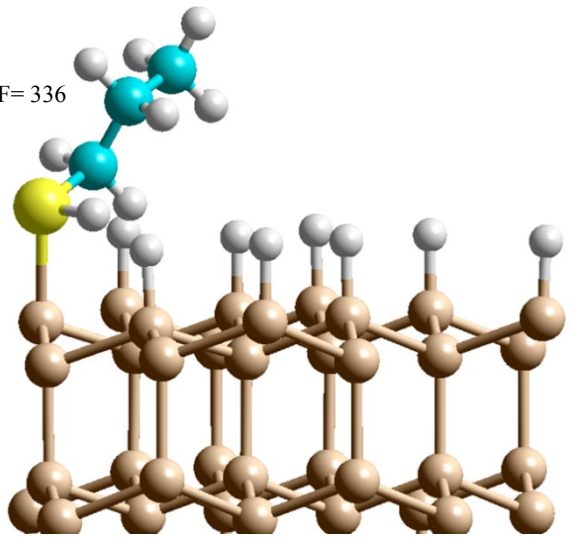
14 16.971882 9.877126 25.238685
14 9.318983 9.871774 25.248394
14 1.668513 1.034603 28.358865
14 5.491394 3.243456 25.245242
14 15.061482 6.552707 25.218236
14 3.580712 4.356943 28.349647
14 5.493139 1.034566 26.012861
14 3.582181 2.148475 29.133083
14 7.404009 4.348974 26.014619
14 5.487452 7.663117 25.991587
14 5.494607 5.463409 29.132731
14 13.146818 9.877443 25.235712
14 5.496955 1.035978 28.359296
14 3.597594 2.155068 1.479786
14 9.317071 3.246182 25.245720
14 7.408952 6.557759 25.245444
14 7.407660 4.351009 28.360946
14 5.487330 7.665827 28.335751
14 5.508016 5.473827 1.479750
14 9.318423 1.036751 26.010827
14 7.412508 2.139364 29.142077
14 13.165705 3.247012 2.266591
14 5.513273 3.260056 2.240611
14 9.331151 9.866209 2.151727
14 11.231290 4.349394 26.013695
14 9.321218 7.663235 26.017159
14 9.324686 5.455811 29.138218
14 7.397222 8.762566 29.128892
14 15.076935 6.572923 2.254537
14 7.425071 6.558738 2.259247
14 9.324567 1.035777 28.357198
14 7.423790 2.144227 1.490409
14 11.229516 6.556343 25.238821
14 11.240113 4.353369 28.359979
14 9.326940 7.668736 28.363483
14 9.336953 5.456733 1.484908
14 7.397082 8.758965 1.472800
14 15.091236 6.591990 4.597374
14 7.433296 6.558470 4.604354
14 11.238881 2.142034 29.141586
14 9.339030 3.248381 2.259941
14 13.153910 9.888191 2.292966
14 7.439763 4.355333 5.381008
14 13.151444 7.661435 25.983796
14 13.153108 5.466738 29.136787
14 11.257556 8.764107 29.130858
14 11.253044 6.559541 2.254301
14 5.531969 7.663226 5.391115
14 9.350698 7.662121 5.348108
14 11.250747 2.143942 1.490115
14 9.343612 3.247415 4.604701

14 13.162014 7.666796 28.328179
14 13.165037 5.459254 1.487335
14 11.267510 8.765506 1.477362
14 11.265036 6.558186 4.597524
14 9.355441 1.058089 5.414751
14 11.247028 4.356851 5.380604
14 15.063493 8.769769 29.140716
14 13.169415 7.650740 5.399433
14 15.069413 8.781875 1.492862
14 1.743326 1.033044 5.244644
14 9.347004 9.822910 4.459355
14 13.184406 3.284801 4.623547
14 5.465239 1.055265 5.191620
14 3.622587 4.391413 5.370526
14 5.519665 3.292048 4.580181
14 13.188662 9.868230 4.663138
14 16.992396 9.873919 4.635515
14 16.989776 9.883237 2.274849
6 1.705039 2.200317 8.594209
6 2.458964 2.808106 9.771524
6 13.416918 4.209184 10.096277
1 13.140609 3.241105 23.741833
1 16.975489 9.890959 23.735030
1 9.320177 9.872005 23.744539
1 5.497832 3.243405 23.741503
1 15.069132 6.540261 23.714787
1 13.147551 9.901292 23.732142
1 9.318842 3.249770 23.742056
1 7.424214 6.550606 23.742028
1 11.212810 6.548908 23.735200
1 7.424305 4.349613 6.884787
1 5.526719 7.638509 6.894659
1 9.348747 7.740931 6.850567
1 9.367150 1.085394 6.919051
1 11.230932 4.371282 6.885496
1 13.166926 7.613269 6.903132
1 5.367318 1.048060 6.705109
1 3.645277 4.384802 6.876966
1 3.517436 0.815331 7.838937
1 1.787037 2.837480 7.701061
1 12.112702 2.096369 8.816806
1 3.531635 2.855423 9.523982
1 2.368543 2.148582 10.648146
1 13.529338 4.883881 9.234879
1 13.962588 4.648851 10.941955
1 12.350035 4.182497 10.362646

---

7. Si(111)-H 3x3 radical, chemisorbed intermediate with C3H7SH

E= -526.1173 eV, Ggas= -518.4443 eV, Gsoln= -518.3644 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 224 NGXF= 126 NGYF= 126 NGZF= 336
Low Frequencies (cm^-1)= -27. 36. 49. 62. 63. 65.



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14 16.960976 9.879856 25.233683
14 9.307251 9.879802 25.233616
14 1.653532 1.042056 28.358411
14 5.480384 3.251469 25.233624
14 15.047507 6.565595 25.233682
14 3.566958 4.356157 28.358386
14 5.480353 1.042031 26.014772
14 3.566964 2.146718 29.139301
14 7.393789 4.356165 26.014751
14 5.480280 7.670384 26.014751

14	5.480357	5.460734	29.139359
14	13.134077	9.879833	25.233643
14	5.480388	1.042073	28.358385
14	3.597594	2.155068	1.479786
14	9.307248	3.251495	25.233658
14	7.393868	6.565604	25.233738
14	7.393852	4.356187	28.358414
14	5.480494	7.670307	28.358725
14	5.508016	5.473827	1.479750
14	9.307241	1.042023	26.014737
14	7.393734	2.146706	29.139254
14	13.165705	3.247012	2.266591
14	5.513273	3.260056	2.240611
14	9.331151	9.866209	2.151727
14	11.220687	4.356177	26.014762
14	9.307251	7.670393	26.014750
14	9.307251	5.460928	29.139318
14	7.393889	8.775160	29.139310
14	15.076935	6.572923	2.254537
14	7.425071	6.558738	2.259247
14	9.307245	1.042161	28.358417
14	7.423790	2.144227	1.490409
14	11.220644	6.565616	25.233678
14	11.220636	4.356206	28.358423
14	9.307239	7.670318	28.358436
14	9.336953	5.456733	1.484908
14	7.397082	8.758965	1.472800
14	15.091236	6.591990	4.597374
14	7.433296	6.558470	4.604354
14	11.220729	2.146747	29.139246
14	9.339030	3.248381	2.259941
14	13.153910	9.888191	2.292966
14	7.439763	4.355333	5.381008
14	13.134119	7.670383	26.014727
14	13.134103	5.460792	29.139295
14	11.220572	8.775216	29.139287
14	11.253044	6.559541	2.254301
14	5.531969	7.663226	5.391115
14	9.350698	7.662121	5.348108
14	11.250747	2.143942	1.490115
14	9.343612	3.247415	4.604701
14	13.134043	7.670331	28.358590
14	13.165037	5.459254	1.487335
14	11.267510	8.765506	1.477362
14	11.265036	6.558186	4.597524
14	9.355441	1.058089	5.414751
14	11.247028	4.356851	5.380604
14	15.047343	8.775361	29.139281
14	13.169415	7.650740	5.399433
14	15.069413	8.781875	1.492862
14	1.743326	1.033044	5.244644
14	9.347004	9.822910	4.459355
14	13.184406	3.284801	4.623547
14	5.465239	1.055265	5.191620
14	3.622587	4.391413	5.370526
14	5.519665	3.292048	4.580181
14	13.188662	9.868230	4.663138
14	16.992396	9.873919	4.635515
14	16.989776	9.883237	2.274849
6	1.619569	2.368757	8.272582
6	2.400430	2.681957	9.541560
6	1.948767	4.021754	10.126947
1	13.132662	3.249238	23.730336
1	16.961246	9.882397	23.730312
1	9.306717	9.877926	23.730343
1	5.480468	3.249183	23.730309
1	15.044241	6.562847	23.730233
1	13.133329	9.878996	23.730415
1	9.307452	3.251141	23.730400
1	7.396568	6.563886	23.730470
1	11.218905	6.564103	23.730466

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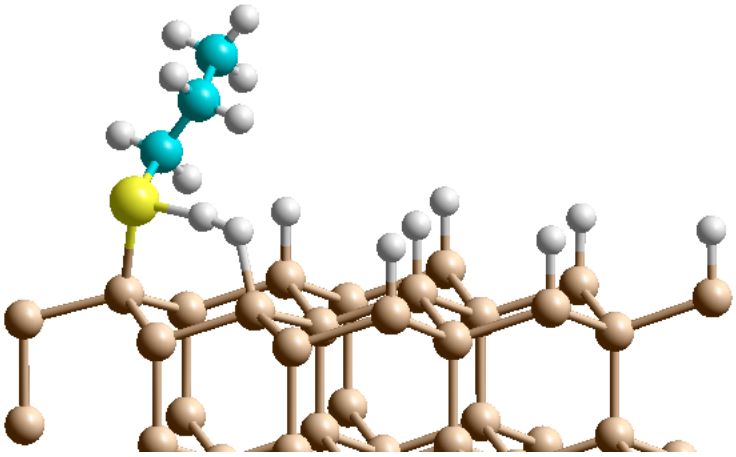
1 5.521149 7.658092 6.897469
1 9.349886 7.755847 6.852570
1 9.378177 1.074012 6.922046
1 11.230457 4.381041 6.887025
1 13.165878 7.613121 6.905037
1 5.329272 1.048177 6.714563
1 3.635677 4.383030 6.880926
1 3.474105 1.072851 7.380199
1 1.742350 3.153516 7.514457
1 12.024532 2.239445 8.460732
1 3.475302 2.723489 9.301980
1 2.266244 1.873266 10.276036
1 13.588735 4.838655 9.408644
1 2.514466 4.256213 11.038174
1 12.361192 4.005117 10.387130

---

8. Si(111)-H 3x3 radical, transition state for chain propagation reaction

E= -525.7470 eV, Ggas= -518.0951 eV, Gsoln= -518.0152 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 224 NGXF= 126 NGYF= 126 NGZF= 336
Low Frequencies (cm^-1)= -901. 6. 29. 46. 61. 72.

16 3.232460 1.364710 14.162920
14 2.613430 3.861800 2.000000
14 2.613430 1.652360 2.781160
14 4.526860 4.966520 2.781160
14 0.700000 0.547640 2.000000
14 4.526860 0.547640 2.000000
14 2.613430 1.652360 5.124620
14 6.440290 3.861800 2.000000
14 4.526860 7.175960 2.000000
14 4.526860 4.966520 5.124620
14 6.440290 1.652360 2.781160
14 4.526860 2.757080 5.905780
14 8.353720 4.966520 2.781160
14 6.440290 8.280680 2.781160
14 6.440290 6.071240 5.905780
14 8.353720 0.547640 2.000000
14 6.440290 1.652360 5.124620
14 4.549140 2.761590 8.244710
14 10.267160 3.861800 2.000000
14 8.353720 7.175960 2.000000
14 8.353720 4.966520 5.124620
14 6.440290 8.280680 5.124620
14 6.463720 6.081930 8.245010
14 10.267160 1.652360 2.781160
14 8.353720 2.757080 5.905780
14 2.635650 3.855880 9.025560
14 6.462710 3.868490 9.007460
14 4.548830 0.531320 8.918560
14 12.180590 4.966520 2.781160
14 10.267160 8.280680 2.781160
14 10.267160 6.071240 5.905780
14 8.353720 9.385400 5.905780
14 4.552680 7.181380 9.020770
14 8.378540 7.167770 9.027610
14 10.267160 1.652360 5.124620
14 8.373760 2.753730 8.255270
14 12.180590 7.175960 2.000000
14 12.180590 4.966520 5.124620
14 10.267160 8.280680 5.124620
14 10.289880 6.065700 8.251950
14 8.353540 9.367420 8.237980
14 4.566730 7.197980 11.363780
14 8.384570 7.162560 11.373550
14 12.180590 2.757080 5.905780



14	10.289420	3.857270	9.027410
14	8.370260	0.555290	9.058610
14	8.392350	4.958570	12.148370
14	14.094020	8.280680	2.781160
14	14.094020	6.071240	5.905780
14	12.180590	9.385400	5.905780
14	12.207810	7.167530	9.021360
14	6.485260	8.270980	12.161120
14	10.304510	8.264970	12.114550
14	12.200040	2.752520	8.254130
14	10.297910	3.854380	11.372370
14	14.094020	8.280680	5.124620
14	14.121070	6.068870	8.251970
14	12.225020	9.373420	8.242800
14	12.222500	7.165540	11.364100
14	10.311800	1.664020	12.181810
14	12.205810	4.961960	12.142020
14	16.007450	9.385400	5.905780
14	14.126460	8.259350	12.164830
14	16.025730	9.389950	8.257030
14	2.697460	1.638940	12.010490
14	4.562720	0.484530	11.227430
14	2.659710	3.888590	11.378300
14	6.424900	1.657080	11.952160
14	4.574530	4.996330	12.132750
14	6.472930	3.894900	11.346740
14	8.403740	0.534520	11.428270
14	0.725310	0.538000	11.397560
14	0.724080	0.548470	9.038830
6	2.756150	2.889200	15.056750
6	3.661800	3.108920	16.264500
6	3.200440	4.308910	17.092380
1	2.618240	3.859180	0.496860
1	0.705520	0.548140	0.496830
1	4.531170	0.546170	0.496870
1	6.444770	3.859140	0.496840
1	4.530770	7.172260	0.496700
1	8.357020	0.546680	0.496920
1	10.271540	3.861090	0.496880
1	8.360920	7.173700	0.496900
1	12.183780	7.174540	0.496910
1	8.370410	4.951770	13.652910
1	6.475530	8.261750	13.665050
1	10.314890	8.347180	13.616030
1	10.326670	1.677450	13.687050
1	12.201300	4.976170	13.647940
1	14.129340	8.233100	13.669610
1	5.877060	1.761940	13.661990
1	4.599670	4.995790	13.639640
1	4.929490	1.681840	13.921940
1	2.808780	3.736330	14.359980
1	1.706270	2.755070	15.353920
1	4.693890	3.266650	15.913710
1	3.676000	2.200830	16.887920
1	3.191840	5.227940	16.489040
1	3.869110	4.473320	17.947970
1	13.665550	4.153540	17.484640

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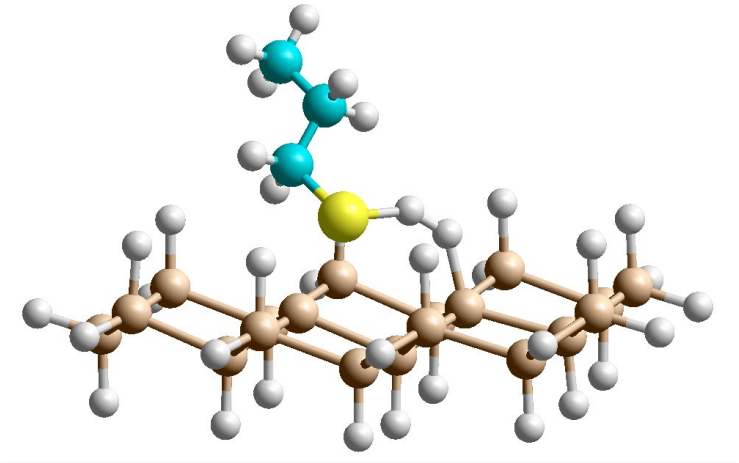
9. Si model compound radical, transition state for chain propagation reaction

#P pbepbe/6-31++g** empiricaldispersion=gd3bj nosym
Full point group C1 NOp 1
SCF Done: E(UPBE-PBE) = -6031.84792005 A.U. after 19 cycles

14	4.489419	-1.613341	11.972749
14	2.639589	-2.767888	11.081333
14	6.449149	-2.762395	11.366665
14	4.528939	0.639077	11.279070
14	2.663200	-4.987559	11.864983



14 0.763992 -1.703279 12.015471
1 2.592856 -2.657802 9.579806
14 8.353402 -1.662095 12.145599
14 6.438855 -4.975197 12.144188
1 6.505912 -2.797708 9.861752
14 2.614312 1.650985 12.144834
14 6.439657 1.651485 12.145366
1 4.530402 0.719559 9.772933
14 4.610112 -6.132438 11.236409
14 0.672389 -6.100817 11.303644
1 2.967452 -4.768661 13.506186
14 0.700059 0.547707 11.378411
14 -1.213682 -2.766499 11.377993
1 0.896547 -1.783830 13.511072
14 8.353581 0.547726 11.378251
1 8.337246 -1.663393 13.649371
1 9.597795 -2.386452 11.710933
1 6.306938 -4.990464 13.641277
1 7.744418 -5.640001 11.803985
1 2.685031 1.535849 13.641338
1 2.587904 3.114974 11.798626
1 6.373309 1.534135 13.643476
1 6.488464 3.115852 11.807454
14 4.526838 -8.289106 12.145512
1 4.760450 -6.209467 9.740627
14 0.700335 -8.288832 12.145549
14 -1.211520 -4.976502 12.145128
1 0.544623 -6.181437 9.802844
1 0.664265 0.616482 9.877418
1 -0.550693 1.204504 11.895537
1 -2.407205 -2.003929 11.886152
1 -1.283468 -2.773225 9.876447
1 9.604585 1.269395 11.799917
1 8.324279 0.524121 9.875670
14 2.613157 -9.395070 11.378131
1 4.459547 -8.152100 13.641159
1 5.773830 -9.062270 11.814341
1 0.728872 -8.224992 13.646668
1 -0.549538 -9.019777 11.739109
1 -1.131446 -4.979463 13.645659
1 -2.460544 -5.713621 11.746585
1 2.618244 -10.838980 11.801522
1 2.616232 -9.364348 9.875197
1 3.431985 -4.053778 14.058223
16 3.906161 -2.440829 14.060093
6 5.467073 -2.477669 15.049055
6 5.328612 -3.392249 16.267461
1 6.289907 -2.814969 14.399423
1 5.671260 -1.437890 15.351782
6 6.609897 -3.380555 17.111504
1 5.109207 -4.419817 15.926591
1 4.465766 -3.070233 16.877130
1 7.476624 -3.730314 16.525255
1 6.507800 -4.040984 17.987552
1 6.838552 -2.365721 17.479001

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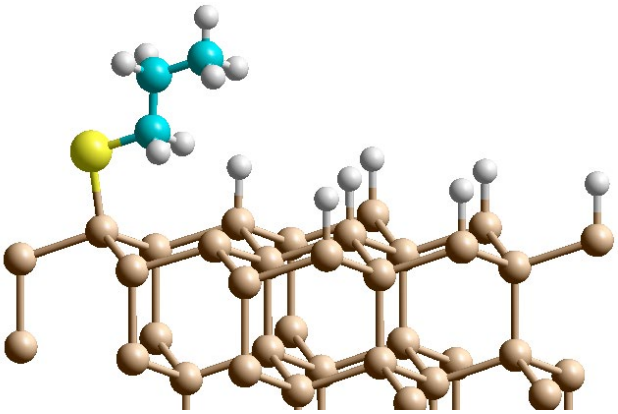
10. Si(111)-H 3x3 radical after first ligand addition

E= -519.7153 eV, Ggas= -512.3831 eV, Gsoln= -512.3032 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 35.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 256 NGXF= 126 NGYF= 126 NGZF= 392
Low Frequencies (cm^-1)= 28. 38. 54. 61. 65. 77.

16 8.134370 4.755680 14.279120
14 8.333550 4.946900 12.147450
14 6.422120 3.858590 11.362730
14 8.341450 7.171000 11.400570
14 10.256440 3.856880 11.375850

14	6.431250	3.862680	9.023210
14	4.521620	4.970660	12.153400
14	6.427250	1.655590	12.151410
14	8.348400	7.175400	9.047220
14	6.428310	8.282580	12.161990
14	10.255200	8.294410	12.138240
14	10.256410	3.863510	9.024860
14	10.256770	1.653390	12.155820
14	12.174500	4.965060	12.070440
14	4.520820	2.756420	8.243340
14	6.436650	6.075110	8.251930
14	8.344770	2.754500	8.246640
14	2.613670	3.862630	11.381630
14	4.517280	7.178450	11.386280
14	4.517330	0.557180	11.367050
14	8.341460	0.550690	11.387540
14	10.276000	6.074920	8.255590
14	8.345190	9.382400	8.252220
14	12.169620	7.181300	11.386170
14	12.174990	2.757980	8.255250
14	4.526860	2.757080	5.905770
14	2.609480	3.860760	9.032070
14	4.519020	0.549240	9.025810
14	6.440290	6.071240	5.905770
14	4.521480	7.176870	9.039610
14	8.353720	2.757080	5.905770
14	8.348360	0.548610	9.039630
14	2.603340	1.653290	12.146910
14	10.267150	6.071240	5.905770
14	12.174270	7.181840	9.033550
14	8.353720	9.385400	5.905770
14	14.084420	8.282630	12.153460
14	12.180590	2.757080	5.905770
14	2.613430	1.652360	5.124620
14	4.526860	4.966520	5.124620
14	6.440290	1.652360	5.124620
14	8.353720	4.966520	5.124620
14	6.440290	8.280680	5.124620
14	10.267150	1.652360	5.124620
14	0.688060	0.547930	11.385820
14	12.180590	4.966520	5.124620
14	10.267150	8.280680	5.124620
14	14.088400	6.072230	8.255740
14	12.176260	9.390190	8.248240
14	2.613430	1.652360	2.781160
14	4.526860	4.966520	2.781160
14	6.440290	1.652360	2.781160
14	8.353720	4.966520	2.781160
14	6.440290	8.280680	2.781160
14	10.267150	1.652360	2.781160
14	0.693970	0.547740	9.039400
14	12.180590	4.966520	2.781160
14	14.094020	6.071240	5.905770
14	10.267150	8.280680	2.781160
14	12.180590	9.385400	5.905770
14	2.613430	3.861800	2.000000
14	0.700000	0.547640	2.000000
14	4.526860	0.547640	2.000000
14	6.440290	3.861800	2.000000
14	4.526860	7.175960	2.000000
14	8.353720	0.547640	2.000000
14	10.267150	3.861800	2.000000
14	8.353720	7.175960	2.000000
14	12.180590	7.175960	2.000000
14	14.094020	8.280680	5.124620
14	14.094020	8.280680	2.781160
14	16.007450	9.385400	5.905770
14	16.001610	9.386020	8.253410
6	11.190480	5.806910	16.898280
6	9.825910	5.330700	16.395370
6	9.781850	5.305440	14.871310



1 11.411990 6.822880 16.539770
1 11.997230 5.147060 16.545820
1 9.605920 4.324310 16.784380
1 9.030680 5.993760 16.771120
1 10.543910 4.616520 14.473290
1 9.987760 6.306200 14.465750
1 4.526630 4.957780 13.654980
1 6.409960 1.650170 13.652200
1 6.421720 8.290220 13.664370
1 10.270710 8.333990 13.641420
1 10.265070 1.658630 13.658490
1 2.617470 1.647610 13.649930
1 14.084590 8.278590 13.656990
1 2.614620 3.860930 0.497110
1 0.701400 0.546360 0.497070
1 4.527200 0.545050 0.497040
1 6.442370 3.862450 0.497050
1 4.528010 7.174190 0.497040
1 8.356720 0.545500 0.497070
1 10.268960 3.860550 0.497100
1 8.355700 7.174030 0.497090
1 12.182060 7.173920 0.497100
1 11.224620 5.823410 17.995930

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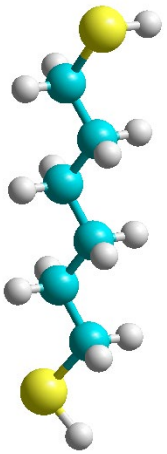
11. HSC6H12SH (**2**)

E= -114.5223 eV
box: 15.000000 0 0 0 15.000000 0 0 0 35.000000
Kpoints: 1 1 1
basis: NGX= 80 NGY= 80 NGZ= 180 NGXF= 160 NGYF= 160 NGZF= 360

16 14.847285 3.798277 16.066160
16 1.534979 10.907950 10.081225
6 0.310345 5.492464 15.577554
6 0.403278 5.718514 14.072060
6 0.720662 7.173314 13.720605
6 0.809941 7.426102 12.215431
6 1.102836 8.888027 11.875648
6 1.185792 9.136509 10.372632
1 14.517588 6.122210 16.012704
1 1.249678 5.769757 16.079987
1 1.180905 5.057090 13.651747
1 14.453325 5.414671 13.601980
1 14.945359 7.830630 14.153423
1 1.671667 7.470012 14.197715
1 1.594869 6.782089 11.780998
1 14.862904 7.119998 11.736939
1 0.316876 9.530345 12.308956
1 2.051054 9.194144 12.350046
1 0.235069 8.869162 9.887890
1 1.988830 8.530199 9.927833
1 0.941817 3.186417 15.564000
1 1.550201 10.856220 8.732436



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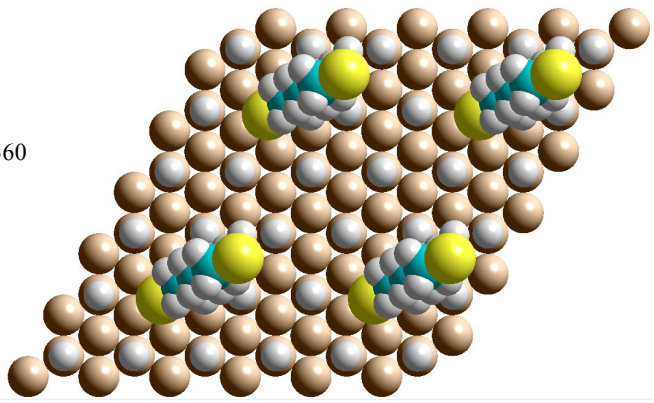
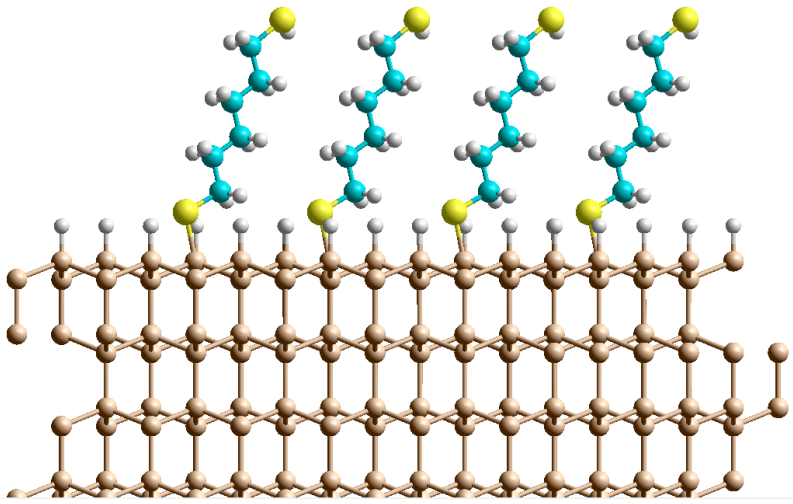
12. Si(111)-H 3x3 1:9 (SiH)8(Si.)0(SiSC6H12SH)1

E= -577.6538 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 35.000000
Kpoints: 2 2 1
basis: NGX= 56 NGY= 56 NGZ= 180 NGXF= 112 NGYF= 112 NGZF= 360

16 12.045706 6.930892 22.427365
16 7.915478 4.754461 14.240244
14 2.613431 3.861800 2.000000
14 2.613431 1.652360 2.781155
14 4.526862 4.966520 2.781155
14 0.700000 0.547640 2.000000



14	4.526862	0.547640	2.000000
14	2.613431	1.652360	5.124620
14	6.440293	3.861800	2.000000
14	4.526862	7.175959	2.000000
14	4.526862	4.966520	5.124620
14	6.440293	1.652360	2.781155
14	4.526862	2.757080	5.905775
14	8.353724	4.966520	2.781155
14	6.440293	8.280679	2.781155
14	6.440293	6.071239	5.905775
14	8.353724	0.547640	2.000000
14	6.440293	1.652360	5.124620
14	4.518328	2.752471	8.244051
14	10.267150	3.861800	2.000000
14	8.353724	7.175959	2.000000
14	8.353724	4.966520	5.124620
14	6.440293	8.280679	5.124620
14	6.439532	6.074661	8.251348
14	10.267150	1.652360	2.781155
14	8.353724	2.757080	5.905775
14	2.608734	3.861154	9.027828
14	6.430702	3.859382	9.013553
14	4.523938	0.544769	9.030268
14	12.180590	4.966520	2.781155
14	10.267150	8.280679	2.781155
14	10.267150	6.071239	5.905775
14	8.353724	9.385399	5.905775
14	4.526849	7.178026	9.041316
14	8.354485	7.173702	9.043115
14	10.267150	1.652360	5.124620
14	8.352901	2.757459	8.251789
14	2.613826	3.862020	11.369732
14	6.419641	3.852793	11.348637
14	4.525745	0.551062	11.372631
14	12.180590	7.175959	2.000000
14	12.180590	4.966520	5.124620
14	10.267150	8.280679	5.124620
14	10.265815	6.069701	8.253282
14	8.350606	9.381723	8.250607
14	4.529697	7.175423	11.388602
14	8.350308	7.172539	11.393649
14	12.180590	2.757080	5.905775
14	10.262179	3.864430	9.048606
14	8.354053	0.550105	9.042917
14	2.612949	1.653897	12.142308
14	4.522028	4.964264	12.148095
14	6.435508	1.653954	12.146782
14	8.321678	4.951481	12.142993
14	14.094020	8.280679	2.781155
14	14.094020	6.071239	5.905775
14	12.180590	9.385399	5.905775
14	12.179992	7.176598	9.035085
14	6.440931	8.280884	12.162909
14	10.267746	8.286317	12.140637
14	12.173010	2.756019	8.253095
14	10.260209	3.859787	11.401997
14	8.351735	0.549835	11.390311
14	0.700075	0.544085	11.384289
14	14.094020	8.280679	5.124620
14	14.095091	6.072163	8.251586
14	12.183148	9.387707	8.251783
14	12.181827	7.177610	11.381379
14	10.268213	1.648360	12.162382
14	12.185406	4.966541	12.142975
14	0.700373	0.545676	9.038628
14	16.007450	9.385399	5.905775
14	14.094931	8.280378	12.151763
14	16.006024	9.386850	8.252688
6	9.392666	5.395651	15.119355
6	9.063168	5.477007	16.605338
6	10.248635	5.930471	17.457602



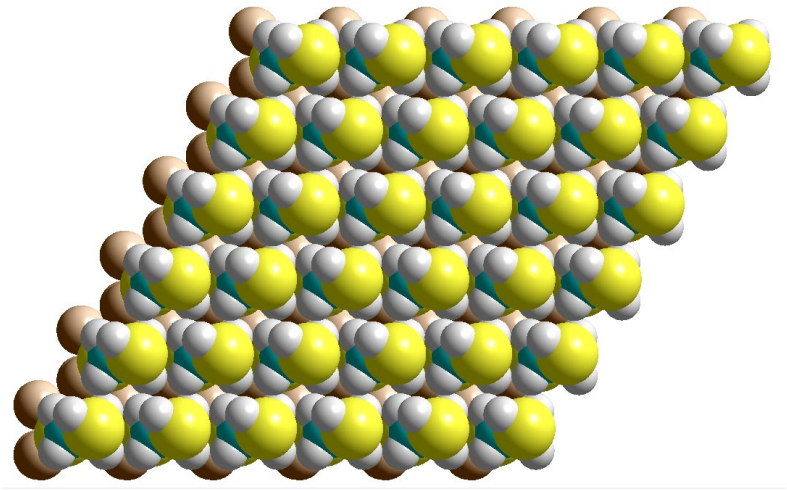
6 9.897556 5.996031 18.944150
6 11.065210 6.431132 19.829767
6 10.679151 6.494091 21.303438
1 10.235082 4.712670 14.937266
1 9.655717 6.384911 14.717378
1 8.719228 4.487857 16.953496
1 8.215204 6.167466 16.750008
1 10.595685 6.921203 17.114889
1 11.096745 5.239225 17.309238
1 9.538013 5.005023 19.274644
1 9.049220 6.689362 19.085875
1 11.427194 7.422477 19.506366
1 11.913612 5.738176 19.706531
1 10.346262 5.505350 21.657536
1 9.840584 7.188641 21.463908
1 12.270545 8.163477 21.921971
1 2.613910 3.862140 0.496800
1 0.699877 0.547448 0.496753
1 4.527758 0.547598 0.496819
1 6.440868 3.861486 0.496801
1 4.526852 7.175133 0.496770
1 8.353582 0.547390 0.496771
1 10.267714 3.862013 0.496807
1 8.354960 7.175736 0.496815
1 12.180765 7.175485 0.496811
1 2.618756 1.656009 13.646519
1 4.518231 4.945445 13.649178
1 6.417938 1.655806 13.647761
1 6.442467 8.290945 13.665346
1 10.279720 8.310389 13.645232
1 10.277949 1.643527 13.665907
1 12.221807 4.968387 13.646435
1 14.088498 8.277552 13.655773

---

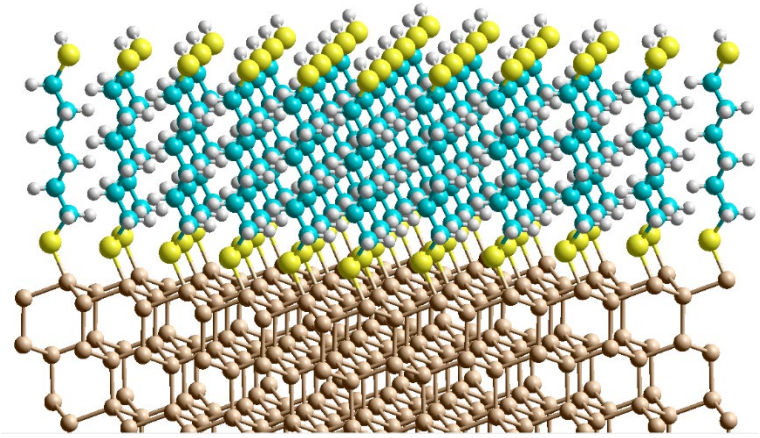
13. Si(111)-H 3x3 1:1 (SiH)0(Si.)0(SiSC6H12SH)9

E=-1442.4569 eV
box: 11.480586 0 0 5.740293 9.942480 0 0 0 35.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 256 NGXF= 126 NGYF= 126 NGZF= 392

16 3.791596 1.422363 14.127922
16 1.213798 1.714808 23.519802
16 7.618458 8.050683 14.127922
16 5.040660 8.343128 23.519802
16 5.705027 4.736523 14.127922
16 3.127229 5.028968 23.519802
16 11.445320 1.422363 14.127922
16 8.867522 1.714808 23.519802
16 15.272182 8.050683 14.127922
16 12.694384 8.343128 23.519802
16 13.358751 4.736523 14.127922
16 10.780953 5.028968 23.519802
16 7.618458 1.422363 14.127922
16 5.040660 1.714808 23.519802
16 11.445320 8.050683 14.127922
16 8.867522 8.343128 23.519802
16 9.531889 4.736523 14.127922
16 6.954091 5.028968 23.519802
14 2.613000 0.548000 2.000000
14 4.527000 1.652000 2.781000
14 4.527000 1.652000 5.125000
14 2.613000 2.757000 5.906000
14 2.598965 2.760735 8.249889
14 2.599045 0.551817 9.032066
14 2.728315 0.537579 11.377204
14 4.642758 1.648473 12.162466
14 6.439862 7.176320 2.000000
14 8.353862 8.280320 2.781000



14	8.353862	8.280320	5.125000
14	6.439862	9.385320	5.906000
14	6.425827	9.389055	8.249889
14	6.425907	7.180137	9.032066
14	6.555177	7.165899	11.377204
14	8.469620	8.276793	12.162466
14	4.526431	3.862160	2.000000
14	6.440431	4.966160	2.781000
14	6.440431	4.966160	5.125000
14	4.526431	6.071160	5.906000
14	4.512396	6.074895	8.249889
14	4.512476	3.865977	9.032066
14	4.641746	3.851739	11.377204
14	6.556189	4.962633	12.162466
14	10.266724	0.548000	2.000000
14	12.180724	1.652000	2.781000
14	12.180724	1.652000	5.125000
14	10.266724	2.757000	5.906000
14	10.252689	2.760735	8.249889
14	10.252769	0.551817	9.032066
14	10.382039	0.537579	11.377204
14	12.296482	1.648473	12.162466
14	14.093586	7.176320	2.000000
14	16.007586	8.280320	2.781000
14	16.007586	8.280320	5.125000
14	14.093586	9.385320	5.906000
14	14.079551	9.389055	8.249889
14	14.079631	7.180137	9.032066
14	14.208901	7.165899	11.377204
14	16.123344	8.276793	12.162466
14	12.180155	3.862160	2.000000
14	14.094155	4.966160	2.781000
14	14.094155	4.966160	5.125000
14	12.180155	6.071160	5.906000
14	12.166120	6.074895	8.249889
14	12.166200	3.865977	9.032066
14	12.295470	3.851739	11.377204
14	14.209913	4.962633	12.162466
14	6.439862	0.548000	2.000000
14	8.353862	1.652000	2.781000
14	8.353862	1.652000	5.125000
14	6.439862	2.757000	5.906000
14	6.425827	2.760735	8.249889
14	6.425907	0.551817	9.032066
14	6.555177	0.537579	11.377204
14	8.469620	1.648473	12.162466
14	10.266724	7.176320	2.000000
14	12.180724	8.280320	2.781000
14	12.180724	8.280320	5.125000
14	10.266724	9.385320	5.906000
14	10.252689	9.389055	8.249889
14	10.252769	7.180137	9.032066
14	10.382039	7.165899	11.377204
14	12.296482	8.276793	12.162466
14	8.353293	3.862160	2.000000
14	10.267293	4.966160	2.781000
14	10.267293	4.966160	5.125000
14	8.353293	6.071160	5.906000
14	8.339258	6.074895	8.249889
14	8.339338	3.865977	9.032066
14	8.468608	3.851739	11.377204
14	10.383051	4.962633	12.162466
6	1.065934	1.575709	15.571918
6	4.065524	1.588832	16.853818
6	1.068331	1.595251	18.139521
6	4.070069	1.591906	19.426843
6	1.068511	1.600538	20.715740
6	4.055968	1.600948	21.987250
6	4.892796	8.204029	15.571918
6	7.892386	8.217152	16.853818
6	4.895193	8.223571	18.139521



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6 5.978955 4.902992 16.853818
6 2.981762 4.909411 18.139521
6 5.983500 4.906066 19.426843
6 2.981942 4.914698 20.715740
6 5.969399 4.915108 21.987250
6 8.719658 1.575709 15.571918
6 11.719248 1.588832 16.853818
6 8.722055 1.595251 18.139521
6 11.723793 1.591906 19.426843
6 8.722235 1.600538 20.715740
6 11.709692 1.600948 21.987250
6 12.546520 8.204029 15.571918
6 15.546110 8.217152 16.853818
6 12.548917 8.223571 18.139521
6 15.550655 8.220226 19.426843
6 12.549097 8.228858 20.715740
6 15.536554 8.229268 21.987250
6 10.633089 4.889869 15.571918
6 13.632679 4.902992 16.853818
6 10.635486 4.909411 18.139521
6 13.637224 4.906066 19.426843
6 10.635666 4.914698 20.715740
6 13.623123 4.915108 21.987250
6 4.892796 1.575709 15.571918
6 7.892386 1.588832 16.853818
6 4.895193 1.595251 18.139521
6 7.896931 1.591906 19.426843
6 4.895373 1.600538 20.715740
6 7.882830 1.600948 21.987250
6 8.719658 8.204029 15.571918
6 11.719248 8.217152 16.853818
6 8.722055 8.223571 18.139521
6 11.723793 8.220226 19.426843
6 8.722235 8.228858 20.715740
6 11.709692 8.229268 21.987250
6 6.806227 4.889869 15.571918
6 9.805817 4.902992 16.853818
6 6.808624 4.909411 18.139521
6 9.810362 4.906066 19.426843
6 6.808804 4.914698 20.715740
6 9.796261 4.915108 21.987250
1 2.613605 0.547448 0.497115
1 1.742480 0.716350 15.542163
1 1.662061 2.485178 15.445841
1 3.405594 0.713847 16.860485
1 3.396723 2.456439 16.841805
1 1.730918 2.467484 18.138277
1 1.735608 0.726522 18.137929
1 4.066529 2.331426 24.224151
1 3.406715 0.720180 19.426618
1 3.400586 2.459127 19.427548
1 1.720167 2.480675 20.717971
1 1.743611 0.737378 20.721405
1 3.447879 0.690711 22.063114
1 3.374450 2.455762 22.007184
1 6.440467 7.175768 0.497115
1 5.569342 7.344670 15.542163
1 5.488923 9.113498 15.445841
1 7.232456 7.342167 16.860485
1 7.223585 9.084759 16.841805
1 5.557780 9.095804 18.138277
1 5.562470 7.354842 18.137929
1 7.893391 8.959746 24.224151
1 7.233577 7.348500 19.426618
1 7.227448 9.087447 19.427548
1 5.547029 9.108995 20.717971
1 5.570473 7.365698 20.721405

1	7.274741	7.319031	22.063114
1	7.201312	9.084082	22.007184
1	4.527036	3.861608	0.497115
1	3.655911	4.030510	15.542163
1	3.575492	5.799338	15.445841
1	5.319025	4.028007	16.860485
1	5.310154	5.770599	16.841805
1	3.644349	5.781644	18.138277
1	3.649039	4.040682	18.137929
1	5.979960	5.645586	24.224151
1	5.320146	4.034340	19.426618
1	5.314017	5.773287	19.427548
1	3.633598	5.794835	20.717971
1	3.657042	4.051538	20.721405
1	5.361310	4.004871	22.063114
1	5.287881	5.769922	22.007184
1	10.267329	0.547448	0.497115
1	9.396204	0.716350	15.542163
1	9.315785	2.485178	15.445841
1	11.059318	0.713847	16.860485
1	11.050447	2.456439	16.841805
1	9.384642	2.467484	18.138277
1	9.389332	0.726522	18.137929
1	11.720253	2.331426	24.224151
1	11.060439	0.720180	19.426618
1	11.054310	2.459127	19.427548
1	9.373891	2.480675	20.717971
1	9.397335	0.737378	20.721405
1	11.101603	0.690711	22.063114
1	11.028174	2.455762	22.007184
1	14.094191	7.175768	0.497115
1	13.223066	7.344670	15.542163
1	13.142647	9.113498	15.445841
1	14.886180	7.342167	16.860485
1	14.877309	9.084759	16.841805
1	13.211504	9.095804	18.138277
1	13.216194	7.354842	18.137929
1	15.547115	8.959746	24.224151
1	14.887301	7.348500	19.426618
1	14.881172	9.087447	19.427548
1	13.200753	9.108995	20.717971
1	13.224197	7.365698	20.721405
1	14.928465	7.319031	22.063114
1	14.855036	9.084082	22.007184
1	12.180760	3.861608	0.497115
1	11.309635	4.030510	15.542163
1	11.229216	5.799338	15.445841
1	12.972749	4.028007	16.860485
1	12.963878	5.770599	16.841805
1	11.298073	5.781644	18.138277
1	11.302763	4.040682	18.137929
1	13.633684	5.645586	24.224151
1	12.973870	4.034340	19.426618
1	12.967741	5.773287	19.427548
1	11.287322	5.794835	20.717971
1	11.310766	4.051538	20.721405
1	13.015034	4.004871	22.063114
1	12.941605	5.769922	22.007184
1	6.440467	0.547448	0.497115
1	5.569342	0.716350	15.542163
1	5.488923	2.485178	15.445841
1	7.232456	0.713847	16.860485
1	7.223585	2.456439	16.841805
1	5.557780	2.467484	18.138277
1	5.562470	0.726522	18.137929
1	7.893391	2.331426	24.224151
1	7.233577	0.720180	19.426618
1	7.227448	2.459127	19.427548
1	5.547029	2.480675	20.717971
1	5.570473	0.737378	20.721405
1	7.274741	0.690711	22.063114

1 7.201312 2.455762 22.007184
1 10.267329 7.175768 0.497115
1 9.396204 7.344670 15.542163
1 9.315785 9.113498 15.445841
1 11.059318 7.342167 16.860485
1 11.050447 9.084759 16.841805
1 9.384642 9.095804 18.138277
1 9.389332 7.354842 18.137929
1 11.720253 8.959746 24.224151
1 11.060439 7.348500 19.426618
1 11.054310 9.087447 19.427548
1 9.373891 9.108995 20.717971
1 9.397335 7.365698 20.721405
1 11.101603 7.319031 22.063114
1 11.028174 9.084082 22.007184
1 8.353898 3.861608 0.497115
1 7.482773 4.030510 15.542163
1 7.402354 5.799338 15.445841
1 9.145887 4.028007 16.860485
1 9.137016 5.770599 16.841805
1 7.471211 5.781644 18.138277
1 7.475901 4.040682 18.137929
1 9.806822 5.645586 24.224151
1 9.147008 4.034340 19.426618
1 9.140879 5.773287 19.427548
1 7.460460 5.794835 20.717971
1 7.483904 4.051538 20.721405
1 9.188172 4.004871 22.063114
1 9.114743 5.769922 22.007184

---

14. Si(111)-H 3x3 8:9 (SiH)0(Si.)1(SiSC6H12SH)8

E=-1330.9651 eV
box: 11.480586 0 0 5.740293 9.942479 0 0 0 30.000000
Kpoints: 2 2 1
basis: NGX= 84 NGY= 84 NGZ= 224 NGXF= 126 NGYF= 126 NGZF= 336

16 4.746504 2.421328 14.119885
16 8.502673 9.134341 14.118100
16 6.702214 5.709213 14.132402
16 16.338723 9.035534 14.177937
16 8.709988 2.362304 14.122511
16 4.553005 1.236377 23.524881
16 14.219294 5.514950 14.200309
16 12.403193 9.050488 14.145829
16 10.483034 5.724764 14.145264
16 7.863686 8.291221 23.564224
16 6.176008 4.724409 23.550312
16 15.559566 7.648576 23.443907
16 8.473691 1.337304 23.577505
16 13.509029 4.037111 23.425192
16 11.771373 8.104290 23.574029
16 9.912711 4.749811 23.557360
14 4.514902 1.576505 12.150290
14 2.583173 0.504931 11.356641
14 2.658659 0.567309 9.016272
14 8.321014 8.242381 12.168001
14 12.153536 1.578430 12.133933
14 2.646005 2.778364 8.253225
14 6.482203 9.396822 8.247471
14 6.421593 7.104159 11.384375
14 10.264309 0.471383 11.337730
14 2.613431 2.757080 5.905775
14 6.440293 9.385399 5.905775
14 6.482994 7.189560 9.037531
14 10.300202 0.548705 9.003791
14 6.430765 4.887273 12.163641
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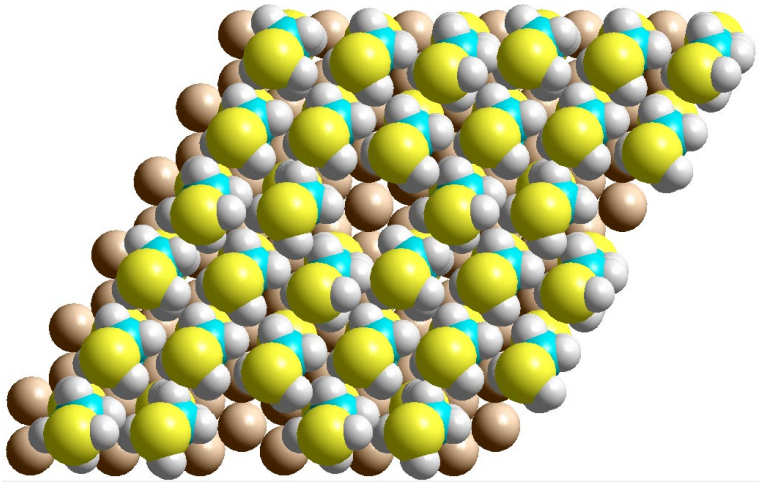
14 8.365784 1.565792 12.148745



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14	12.180586	1.652360	5.124620
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14	16.007448	8.280679	5.124620
14	4.566129	6.086665	8.253308
14	10.303321	2.765802	8.251535
14	14.124315	9.381759	8.246782
14	4.510544	3.791100	11.370033
14	14.086584	7.117183	11.419248
14	6.428386	0.474071	11.383832
14	4.526862	1.652360	2.781155
14	12.180586	1.652360	2.781155
14	10.267155	2.757080	5.905775
14	8.353724	8.280679	2.781155
14	4.526862	6.071239	5.905775
14	16.007448	8.280679	2.781155
14	14.094017	9.385399	5.905775
14	4.569910	3.876714	9.027590
14	14.136194	7.182140	9.059271
14	6.486641	0.559902	9.037529
14	14.078390	4.890986	12.151379
14	12.162578	8.209096	12.177924
14	2.613431	0.547640	2.000000
14	10.267155	0.547640	2.000000
14	8.353724	1.652360	5.124620
14	6.440293	7.175959	2.000000
14	6.440293	4.966519	5.124620
14	14.094017	4.966519	5.124620
14	14.094017	7.175959	2.000000
14	12.180586	8.280679	5.124620
14	12.217541	6.078628	8.263912
14	6.479904	2.767063	8.250639
14	10.311004	9.399137	8.250055
14	12.145586	3.794231	11.425116
14	10.231633	7.131943	11.390841
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14	6.440293	2.757080	5.905775
14	6.440293	4.966519	2.781155
14	14.094017	4.966519	2.781155
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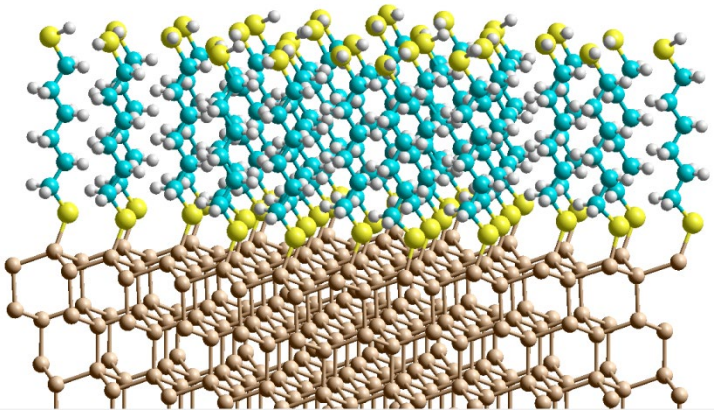
14	6.440293	0.547640	2.000000
14	4.526862	3.861799	2.000000
14	12.180586	3.861799	2.000000
14	10.267155	4.966519	5.124620
14	10.267155	7.175959	2.000000
14	8.393342	6.084153	8.252965
14	8.333735	3.783439	11.375805
14	10.267155	4.966519	2.781155
14	8.353724	6.071239	5.905775
14	8.394402	3.874202	9.032034
14	8.353724	3.861799	2.000000
6	4.385073	1.378778	15.574103
6	4.869575	2.068129	16.843865
6	4.464963	1.345311	18.127658
6	4.918180	2.039678	19.408219
6	8.134990	8.091140	15.563318
6	4.511076	1.327927	20.697266
6	8.415692	8.873163	16.842507
6	5.003523	2.039857	21.946951
6	8.152815	8.096189	18.133973
6	6.393263	4.644921	15.579864
6	15.842016	7.934825	15.542404
6	8.362309	1.294609	15.562060
6	8.373204	8.916563	19.404887
6	6.824525	5.373237	16.849083
6	16.273788	8.573156	16.857441



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6	16.243634	8.462930	19.398370
6	12.445211	8.714286	16.863074
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6	8.519324	1.219697	20.704053
6	6.794262	5.408862	21.985905
6	14.116858	4.777303	19.328431
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6	16.234180	8.423196	21.934419
6	12.467757	8.703878	19.434007
6	9.159751	1.805250	21.957227
6	13.711050	4.035275	20.602111
6	10.193029	4.617052	18.139086
6	11.963940	8.043668	20.720245
6	14.107280	4.779551	21.873459
6	10.590808	5.338961	19.424934
6	12.465062	8.700630	22.002007
6	10.179932	4.622977	20.711943
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15. Si(111)-H 3x3 8:9 (SiH)1(Si.)0(SiSC6H12SH)8

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16 13.503294 4.029579 23.422043
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14 12.151258 1.606728 12.168371
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14 6.477779 9.397840 8.247765
14 6.420291 7.103389 11.385021
14 10.267229 0.478335 11.348461
14 2.613431 2.757080 5.905775
14 6.440293 9.385399 5.905775
14 6.476806 7.191337 9.038470
14 10.299286 0.554631 9.014924
14 6.425289 4.885717 12.161677
14 16.016872 8.231986 12.190889
14 8.359613 1.563812 12.149402
14 4.526862 1.652360 5.124620
14 12.180586 1.652360 5.124620
14 8.353724 8.280679 5.124620
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14 4.559655 6.089318 8.253226
14 10.295121 2.767699 8.247931
14 14.124981 9.387614 8.249931
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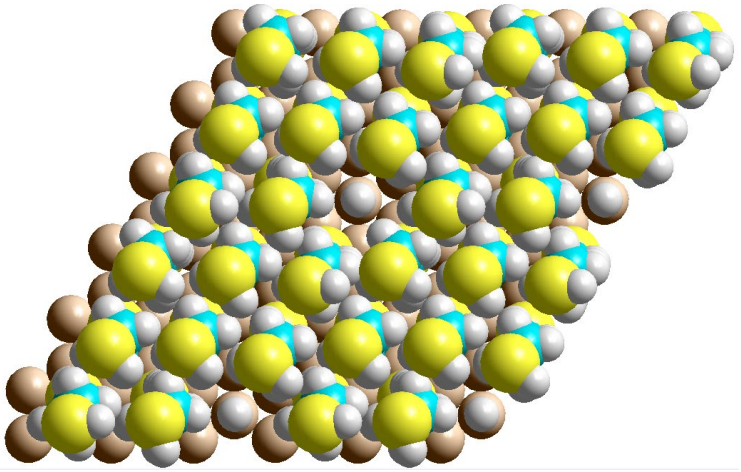

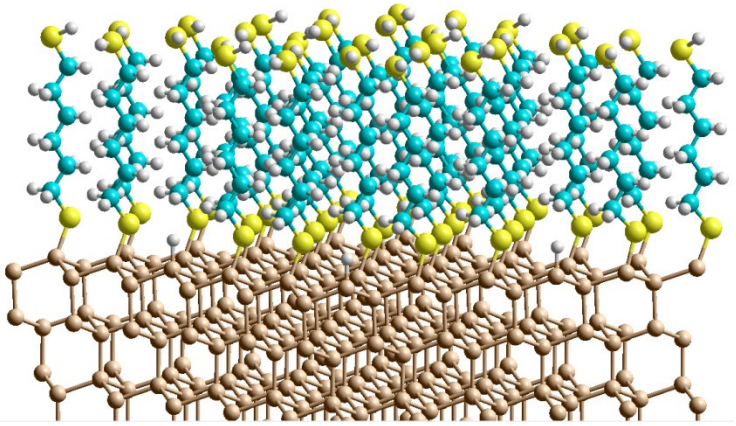

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16. Si(111)-H 3x3 7:9 (SiH)1(Si.)1(SiSC6H12SH)5

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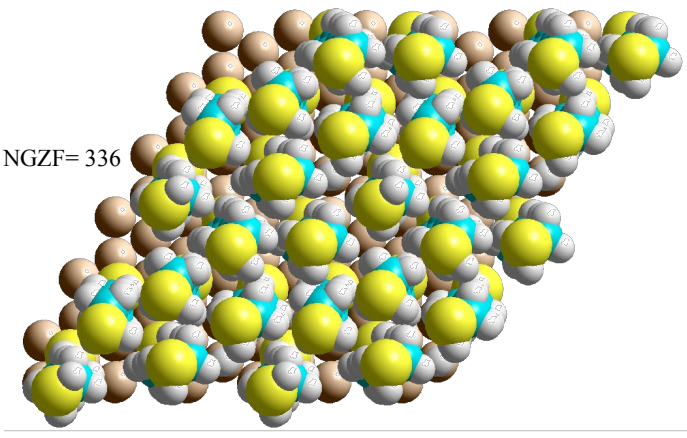

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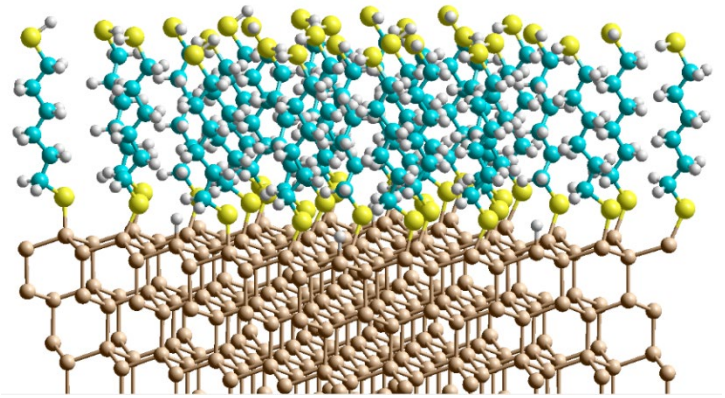

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17. Si(111)-H 3x3 2:3 (SiH)2(Si.)1(SiSC6H12SH)6

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16 9.717618 9.190315 22.980938
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14 2.668540 0.564605 9.042602
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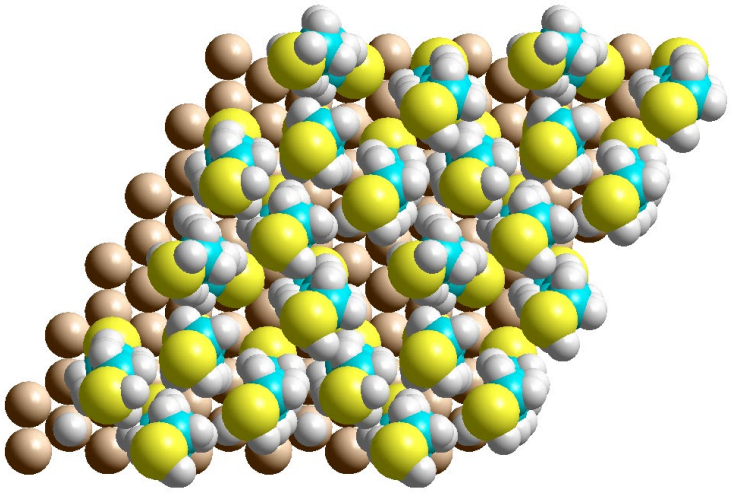

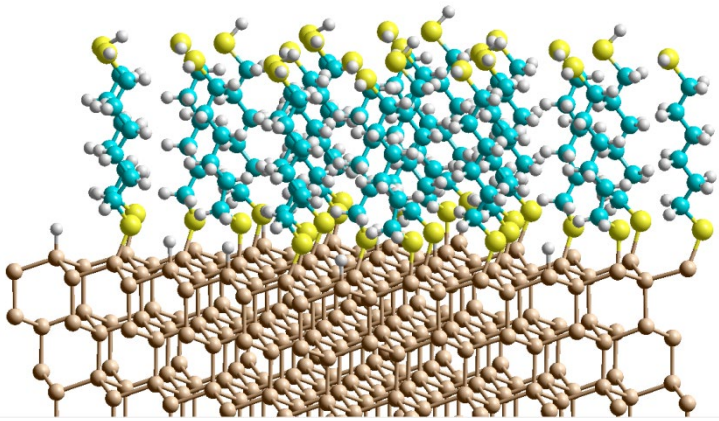

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1	11.597775	4.069225	18.147310
1	9.859718	4.305256	18.209486
1	5.221282	5.634854	23.415714
1	10.118030	8.277428	20.202357
1	9.095881	9.700599	20.279655
1	9.841831	-0.380533	23.504214
1	3.653291	3.330975	21.902171
1	13.641032	4.240228	21.695656
1	11.930102	6.218937	19.412577
1	10.194779	6.518687	19.342157
1	6.039313	-0.677908	21.733046
1	5.223012	0.892107	21.700673
1	2.397342	1.188348	22.969470
1	11.439767	4.092816	20.757324
1	9.729948	4.469096	20.658985
1	10.381127	9.798712	23.983550

1	11.841029	6.170648	22.107074
1	10.159198	6.655155	21.894502
1	11.129221	3.900055	23.409844
1	12.190788	1.611226	13.634529
1	6.712127	3.265806	14.907377
1	7.924605	4.728603	16.544840
1	7.095134	2.666642	17.620751
1	7.974851	4.518599	19.117361
1	7.265341	2.430734	20.326566
1	7.969877	4.385062	21.743188
1	7.617371	3.366114	23.791800
1	4.637755	1.587170	13.659987

10. Silicon STM tip preparation

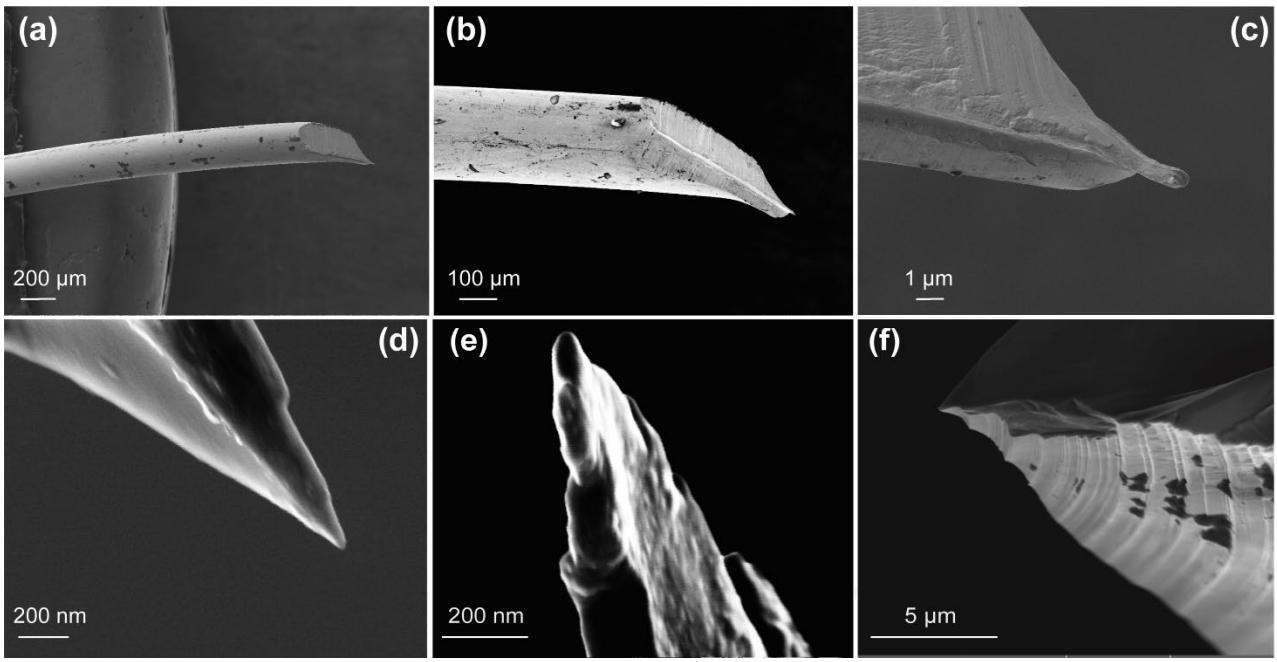

Figure S14. (a-c) SEM images of mechanically cut gold STM tips at different scales. The radius of these conventional gold tips is comparable to that formed with silicon (111) tips shown in (d-f). SEM images of typical silicon (111) tips prepared by etching in 3.50 M KOH solution for 48 h at 65 °C. The tip preparation procedure consistently led to tip radii less than 1 µm and is comparable to that of gold STM tips.