Electronic supplementary information (ESI)

Origin of Humidity Influencing the Excited State Electronic Properties of Silicon Quantum Dots based Light-emitting Diodes

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Section 1. The absorption spectrum of Si QDs

The molecular structures including H-passivated Si QDs with one hydrogen atom replaced by fluorine atom (Si-F), hydroxyl group (Si-OH) and a silicon-oxygen double bond (Si=O) were used in this work, respectively.[1-4] Ambient conditions are vacuum or the presence of 1-5 water molecules. In the case of the absorption spectra of Si-H, Si-F, and Si-OH, the excitation wavelengths are mainly concentrated at 250 nm ~ 300 nm.[5] In addition, the highest absorption peak of Si-H is in five water molecules, while Si-F is in three water molecules. For the absorption spectra of Si-Si=O, the excitation wavelengths are near 300 nm with the highest absorption peak in vacuum. All in all, it can be shown that the presence of water in the F, OH, and Si=O functional groups has little effect on the absorption spectrum.

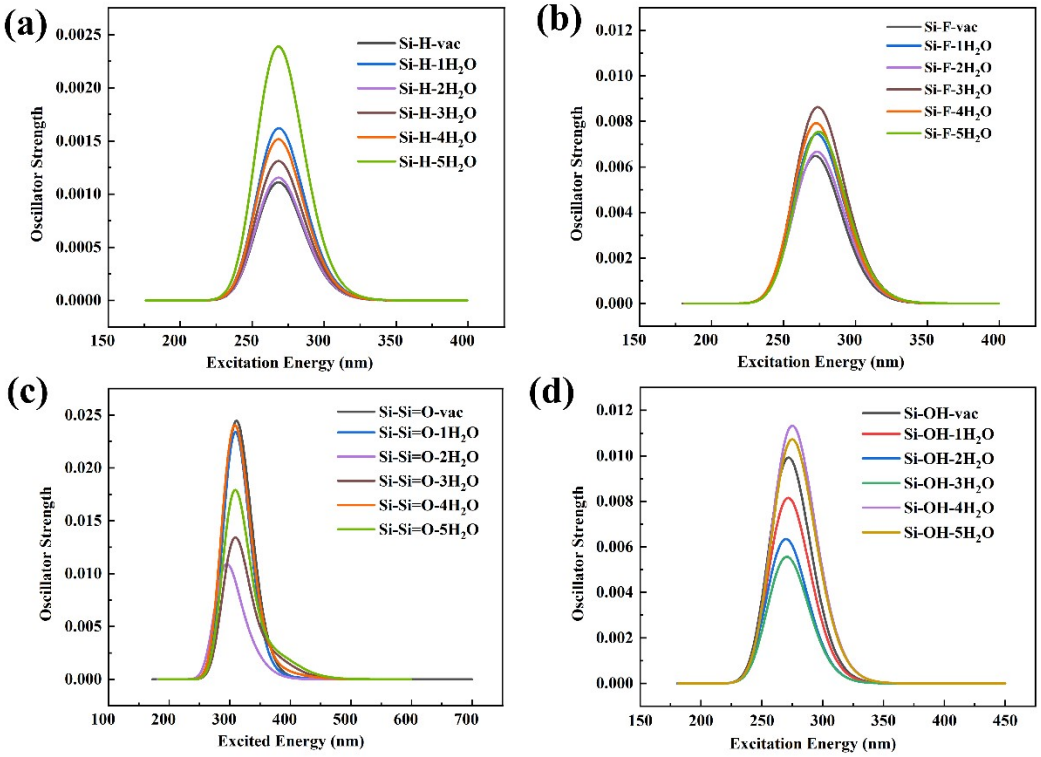

Figure S1. Absorption spectra of (a) $Si_{29}H_{36}$ (Si-H), (b) $Si_{29}H_{36}$ cluster with a hydrogen atom replaced by F group (Si-F), (c) $Si_{29}H_{36}$ cluster passivated with the substituent group of a silicon-oxygen double bond (Si=O), and (d) $Si_{29}H_{36}$ cluster with a hydrogen atom replaced by OH group (Si-OH) under the vacuum environment and the water vapor environment including one to five water molecules in the vicinity of the passivated functional groups. The upper right corner clearly identifies the environment in which each system is located. For example, Si-F-$1H_2O$ indicates that the silicon cluster with the F group is in the environment of one water molecule.

Section 2. Absorption wavelength and emission wavelength

In both the water and vacuum environment, the excitation wavelength of Si-H is concentrated around 269 nm; the excitation wavelength of Si29-F focus on 274~278 nm; the excitation wavelength of Si-F focus on 270~280 nm. In vacuum, the excitation wavelength of Si-Si=O is 413 nm. The excitation wavelength of Si29-Si=O is decreased in the water environment.

Table S1. Absorption wavelengths (EX) of Si-H, Si-F, Si-OH, and Si-Si=O in the water and vacuum environment. Absorption wavelength in nm (eV). In the first column, the surface termination conditions and the environment of the silicon quantum dots are briefly indicated. For example, Si-F-1H_2O indicates that the silicon cluster with F group is in the environment of 1 water molecule.

System	EX in nm (eV)	System	EX in nm (eV)
Si-H-vac	269 (4.6)	Si-OH-vac	274 (4.5)
Si-H-1H_2O	269 (4.6)	Si-OH-1H_2O	274 (4.5)
Si-H-2H_2O	269 (4.6)	Si-OH-2H_2O	272 (4.6)
S-H-3H_2O	269 (4.6)	Si-OH-3H_2O	273 (4.6)
Si-H-4H_2O	269 (4.6)	Si-OH-4H_2O	279 (4.4)
Si-H-5H_2O	267(4.6)	Si-OH-5H_2O	279 (4.4)
Si-F-vac	275 (4.5)	Si-Si=O-vac	413 (3.0)
Si-F-1H_2O	276 (4.5)	Si-Si=O-1H_2O	395 (3.1)
Si-F-2H_2O	276 (4.5)	Si-Si=O-2H_2O	329 (3.8)
Si-F-3H_2O	276 (4.5)	Si-Si=O-3H_2O	371(3.3)
Si-F-4H_2O	275 (4.5)	Si-Si=O-4H_2O	371 (3.3)
Si-F-5H_2O	277 (4.5)	Si-Si=O-5H_2O	379 (3.3)

Table S2. Emission wavelengths (EM) of Si-H, Si-F, Si-OH, and Si-Si=O in the water and vacuum environment. Emission wavelength (EM) in nm (eV). In the first column, the surface termination conditions and the environment of the silicon quantum dots are briefly indicated. For example, Si-F-$1H_2O$ indicates that the silicon cluster with the F group is in the environment of 1 water molecule.

System	EM in nm (eV)	System	EM in nm (eV)
Si-H-vac	512 (2.4)	Si-OH-vac	496 (2.5)
Si-H-$1H_2O$	508 (2.4)	Si-OH-$1H_2O$	504 (2.5)
Si-H-$2H_2O$	520 (2.4)	Si-OH-$2H_2O$	495 (2.5)
Si-H-$3H_2O$	518 (2.4)	Si-OH-$3H_2O$	505 (2.5)
Si-H-$4H_2O$	505 (2.4)	Si-OH-$4H_2O$	828 (1.5)
Si-H-$5H_2O$	516 (2.4)	Si-OH-$5H_2O$	889 (1.4)
Si-F-vac	510 (2.4)	Si-Si=O-vac	862 (1.4)
Si-F-$1H_2O$	501 (2.5)	Si-Si=O-$1H_2O$	821 (1.5)
Si-F-$2H_2O$	495 (2.5)	Si-Si=O-$2H_2O$	853 (1.5)
Si-F-$3H_2O$	510 (2.4)	Si-Si=O-$3H_2O$	800 (1.5)
Si-F-$4H_2O$	504 (2.5)	Si-Si=O-$4H_2O$	807 (1.5)
Si-F-$5H_2O$	515 (2.4)	Si-Si=O-$5H_2O$	809 (1.5)

Section 3. Distribution of electrons and holes in the ground state structure

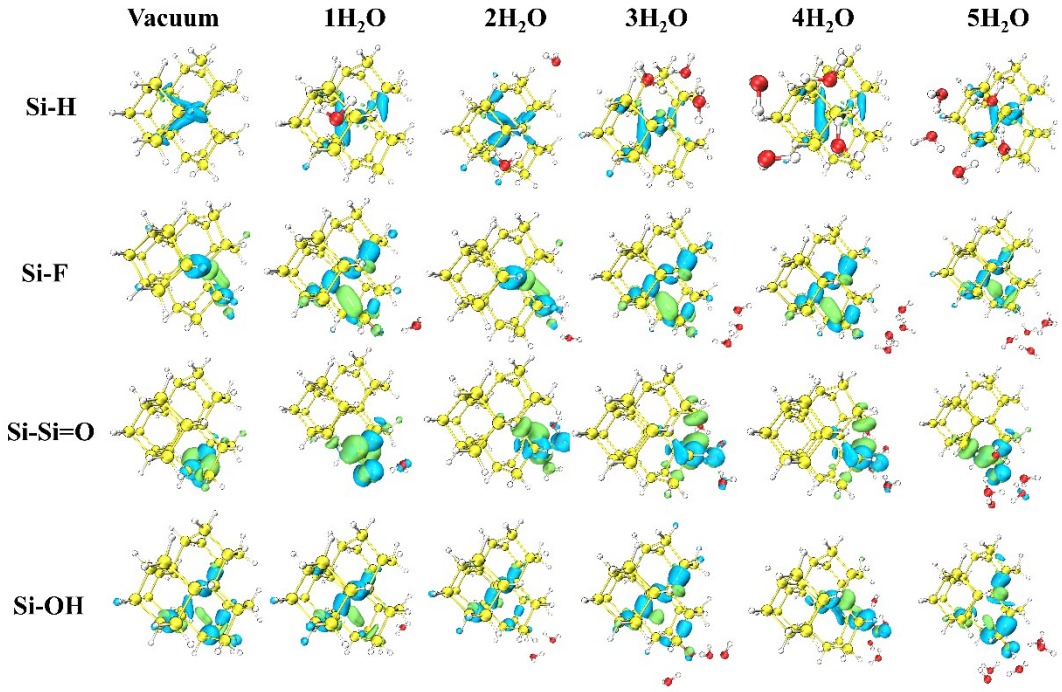

Figure S2. Distribution of electrons and holes in the ground state structure. The Si-H, Si-F, Si-OH, and Si=O groups under vacuum environment and one to five water molecules absorbed around the corresponding functional groups. The green and blue colors with the isosurface value of ±0.002 represent the distribution of electrons and holes, respectively. The silicon, hydrogen, oxygen, and fluorine atom are colored by grey, white, red, and cyan-blue spheres, respectively.

For the electron-hole distribution analysis of the ground state structure, the electron-hole distribution of Si-OH with $4H_2O$ or $5H_2O$ is still in a dispersed state.

Section 4. The D-index, Sr-index, t-index, and Δσ index were obtained by electron-hole analysis of excited state structure

Table S3. The D-index, Sr-index, t-index, and Δσ index were obtained by electron-hole analysis of excited state structure. The D-index measures the distance between the hole and the electronic centroid. The Sr-index is a function of overlap between electron and hole distribution, The larger these two indices are, the higher the degree of overlap between holes and electrons is. The Δσ index reflects the difference in the overall spatial distribution of electrons and holes. The t-index measures the degree of separation of holes and electrons. The above data are all related to S1 of Si QDs in excited states.

System	D-index (Å)	Sr-index (a.u)	Δσ index	t-index (Å)
Si-H-vac	1.8	0.3	0.1	0.2
Si-H-1H_2O	2.7	0.3	0.1	0.8
Si-H-2H_2O	1.8	0.3	0.1	0.2
Si-H-3H_2O	1.8	0.3	0.1	-0.1
Si-H-4H_2O	2.7	0.3	0.1	1.4
Si-H-5H_2O	1.7	0.3	0.1	-0.1
Si-F-vac	1.9	0.3	0.1	0.1
Si-F-1H_2O	2.1	0.4	0.2	0.3
Si-F-2H_2O	2.0	0.4	0.2	-0.1
Si-F-3H_2O	2.0	0.3	0.1	0.3
Si-F-4H_2O	1.9	0.3	0.2	0.1
Si-F-5H_2O	2.0	0.3	0.1	0.3
Si-OH-vac	1.9	0.5	0.2	0.1
Si-OH-1H_2O	2.1	0.5	0.2	0.3
Si-OH-2H_2O	1.9	0.5	0.2	0.1
Si-OH-3H_2O	2.0	0.5	0.2	-0.1
Si-OH-4H_2O	2.5	0.5	0.4	0.7
Si-OH-5H_2O	3.0	0.4	0.6	1.3
Si-Si=O-vac	0.4	0.6	-0.2	-0.7
Si-Si=O-1H_2O	0.4	0.6	-0.4	-1.0
Si-Si=O-2H_2O	0.4	0.6	-0.3	-1.2
Si-Si=O-3H_2O	0.4	0.6	-0.5	-0.8
Si-Si=O-4H2O	0.5	0.6	-0.5	-1.1
Si-Si=O-5H_2O	0.6	0.6	-0.3	-1.0

Table S4. The Δr index and Λ index of excited state structures. Δr index measures the centroid distance of holes and electrons, which is similar to the D index. Λ index measures the degree of overlap of two orbits, which is similar to the Sr index.

System	Δr index	Λ index	System	Δr index	Λ index
Si29-H-vac	3.7	0.34	Si29-OH-vac	3.7	0.5
Si29-H-1H_2O	5.2	0.28	Si29-OH-1H_2O	4.2	0.4
Si29-H-2H_2O	3.8	0.33	Si29-OH-2H_2O	3.7	0.5
Si29-H-3H_2O	3.8	0.34	Si29-OH-3H_2O	4.1	0.5
Si29-H-4H_2O	5.1	0.28	Si29-OH-4H_2O	4.9	0.4
Si29-H-5H_2O	3.6	0.35	Si29-OH-5H_2O	5.9	0.4
Si29-F-vac	3.9	0.34	Si29-Si=O-vac	1.2	0.6
Si29-F-1H_2O	4.2	0.44	Si29-Si=O-1H_2O	1.3	0.6
Si29-F-2H_2O	4.1	0.45	Si29-Si=O-2H_2O	1.2	0.6
Si29-F-3H_2O	4.2	0.33	Si29-Si=O-3H_2O	1.6	0.6
Si29-F-4H_2O	3.9	0.33	Si29-Si=O-4H_2O	1.5	0.6
Si29-F-5H_2O	4.3	0.33	Si29-Si=O-5H_2O	1.6	0.6

Meaning of related characters

Density distribution of hole and electron applied to TDHF and TDDFT cases can be defined as:[6-8]

$$\rho^{hole}(r) = \rho^{hole}_{(loc)}(r) + \rho^{hole}_{(cross)}(r)$$

$$\rho^{hole}_{(loc)}(r) = \sum_{i\to a}(w_i^a)^2\varphi_i\varphi_i - \sum_{i\leftarrow a}(w'^a_i)^2\varphi_i\varphi_i$$

$$\rho^{hole}_{(cross)}(r) = \sum_{i\to a}\sum_{j\neq i\to a} w_i^a w_j^a\varphi_i\varphi_j - \sum_{i\leftarrow a}\sum_{j\neq i\leftarrow a} w'^a_i w'^a_j\varphi_i\varphi_j$$

$$\rho^{ele}(r) = \rho^{ele}_{(loc)}(r) + \rho^{ele}_{(cross)}(r)$$

$$\rho^{ele}_{(loc)}(r) = \sum_{i\to a}(w_i^a)^2\varphi_i\varphi_i - \sum_{i\leftarrow a}(w'^a_i)^2\varphi_i\varphi_i$$

$$\rho^{ele}_{(cross)}(r) = \sum_{i\to a}\sum_{i\to b\neq a} w_i^a w_i^b\varphi_a\varphi_b - \sum_{i\leftarrow a}\sum_{i\leftarrow b\neq a} w'^a_i w'^b_i\varphi_a\varphi_b$$

note that the notions used here:

$$\sum_{i\to a} \equiv \sum_{i}^{occ}\sum_{a}^{vir} \qquad \sum_{i\to a}\sum_{j\neq i\to a} \equiv \sum_{i}^{occ}\sum_{j\neq i}^{occ}\sum_{a}^{vir}$$

where **r** and φ denote coordinate vector and molecular orbitals (MOs) wavefunction. *i/j* and *a/b* respectively are occupied and virtual MOs. *w* and *w'* is known as the configuration coefficient of excitation and de-excitation, respectively. "loc" and "cross" stand for the contribution of local term and cross term to the hole and electron distribution, respectively. Note that the definition of hole and electron given above is in density form rather than wavefunction form, hence the hole and electron do not have phase.

To characterize overlapping extent of hole and electron, S_m index and S_r index are defined as follows:

$$S_m\ index = \int S_m(r)dr \equiv \int min[\rho^{hole}(r), \rho^{ele}(r)]dr$$

$$S_r\ index = \int S_r(r)dr \equiv \int \sqrt{\rho^{hole}(r)\rho^{ele}(r)}dr$$

Note that S_r index must be equal or larger than S_m index.

Centroid can be calculated to reveal most representative position of hole and electron distribution. For instance, X coordinate of centroid of electron is denoted as:

$$X_{ele} = \int x\,\rho^{ele}(r)\,dr$$

where *x* is X component of position vector **r**.

The charge transfer (CT) length in X/Y/Z can be measured by distance between centroid of hole and electron in corresponding directions:

$$D_x = |X_{ele} - X_{hole}|$$

$$D_y = |Y_{ele} - Y_{hole}|$$

$$D_z = |Z_{ele} - Z_{hole}|$$

Therefore, *D* index can be denoted as the total magnitude of CT length shown as:

$$D\ index = |D| = \sqrt{(D_x)^2 + (D_y)^2 + (D_z)^2}$$

The RMSD of hole and electron can be used to characterize their extent of spatial distribution. For example, X component of RMSD of hole can be expressed as:

$$\sigma_{hole,\,x} = \sqrt{\int (x - X_{hole})^2\rho^{hole}(r)dr}$$

The $|\sigma_{hole}|$ and $|\sigma_{hole}|$ are referred as σ_{hole} and σ_{hole} indices, and they measure overall RMSD of hole and electron, respectively.

The difference between RMSD of electron and hole in X/Y/Z direction can be measured via $\Delta\sigma_{\lambda}$, while overall difference can be measured by $\Delta\sigma$ index

$\Delta\sigma_{\lambda} = \sigma_{ele,\lambda} - \sigma_{hole,\lambda} \ \ \lambda = \{x,y,z\}$

$\Delta\sigma \ index = |\sigma_{ele}| - |\sigma_{hole}|$

H_{λ} measures average degree of spatial extension of hole and electron distribution in X/Y/Z direction, H_{CT} is that in CT direction, and *H* index is an overall measure.

$H_{\lambda} = (\sigma_{ele,\lambda} - \sigma_{hole,\lambda})/2 \ \ \lambda = \{x,y,z\}$

$H_{CT} = |H \cdot u_{CT}|$

$H \ index = (|\sigma_{ele}| + |\sigma_{hole}|)/2$

where $\mathbf{u}_{CT}$ is the unit vector in CT direction and can be straightforwardly derived using the centroid of hole and electron.

t index is designed to measure the separation degree of hole and electron in CT direction:

$t \ index = D \ index - H_{CT}$

If *t* index is smaller than 0, it implies that hole and electron is not substantially separated due to CT. Clear separation of hole and electron distributions must correspond to evidently positive *t* index.

The exciton binding energy describe the Coulomb attractive energy between electron and hole, which can be calculated by simple Coulomb formula as follows:

$$E_c = \iint \frac{\rho^{hole}(r_1)\rho^{ele}(r_2)}{|r_1 - r_2|} dr_1 dr_2$$

Excitation type

Electron excitations are classified in different ways. For the electron excitation category involved in UV-Vis spectrum, it can be divided into two categories:

(1) Valence shell excitation: electrons are excited from valence shell occupied orbitals to valence shell empty orbitals. The valence orbital referred to a molecular orbital composed of a mixture of valence atomic orbitals.

(2) Rydberg excitation: electrons are excited from the valence shell occupied orbital to the Rydberg orbital. Rydberg orbitals are those empty orbits that are very diffuse. Such orbitals usually do not exhibit molecular orbital characteristics, but the overall shape exhibits atomic orbital characteristics.

Valence layer excitation can be further divided into

(1) Local excitation (LE): the distribution area of electrons does not change significantly before and after excitation. LE excitation can be classified as a metal-centered transition (MC), intraligand or ligand-centered transition (LC).

(2) Charge-transfer excitation (CT): After the electrons are excited, the distribution area is significantly transferred. It can be transferred both intramolecularly and intermolecularly. CT excitation can be classified into metal-to-metal charge transfer (MMCT), ligand-to-ligand charge transfer (LLCT), metal-to-ligand charge transfer (MLCT), and ligand-to-metal charge transfer (LMCT). For example, MLCT

represents the transfer of excited electrons from the metal to the ligand.

Section 5. Electronic transition orbitals in excited states

Below are the LUMO and HOMO orbital diagrams of the investigated silicon clusters. $Si_{29}H_{36}$ (Si-H), $Si_{29}H_{36}$ cluster with a hydrogen atom replaced by F group (Si-F), $Si_{29}H_{36}$ cluster passivated with the substituent group of a silicon-oxygen double bond (Si=O), $Si_{29}H_{36}$ cluster with a hydrogen atom replaced by OH group (Si-OH) under the vacuum environment and the water vapor environment including one to five water molecules in the vicinity of the passivated functional groups.

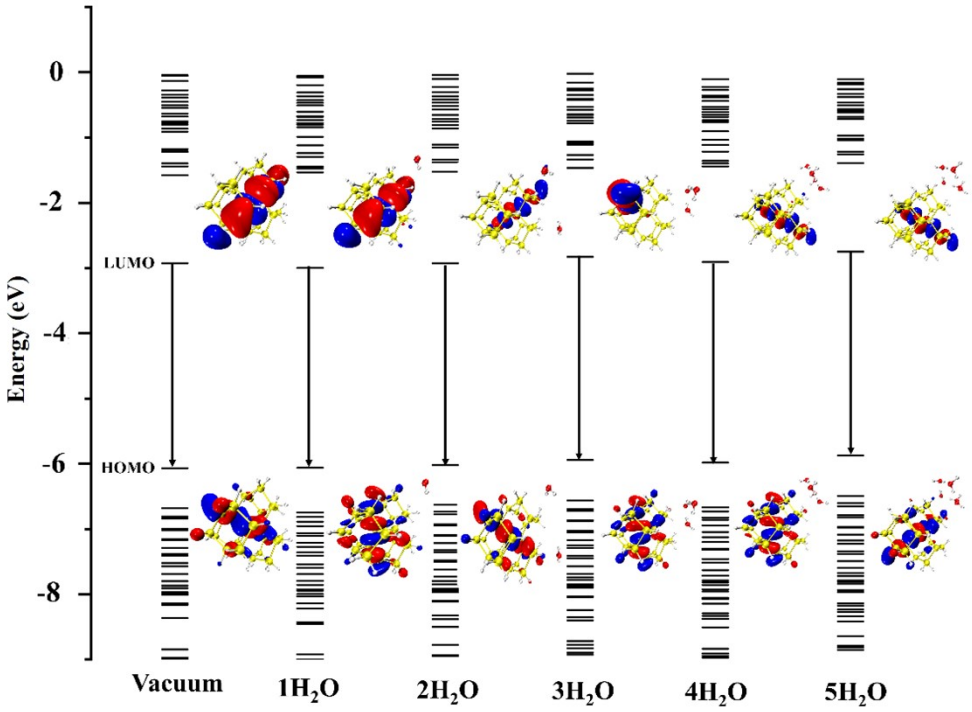

Figure S3a. Electronic transition orbits in excited states for Si-H in vacuum and the presence of one to five water molecules. Wave function isosurfaces are controlled at the same isovalue. The positive and negative phase parts of the orbital wave function are presented in red and blue, respectively. The thick arrows indicate electronic transitions of the excited state. The Si QDs ($Si_{29}H_{36}$) are presented in yellow. The oxygen and hydrogen atoms are shown in red, and white, respectively.

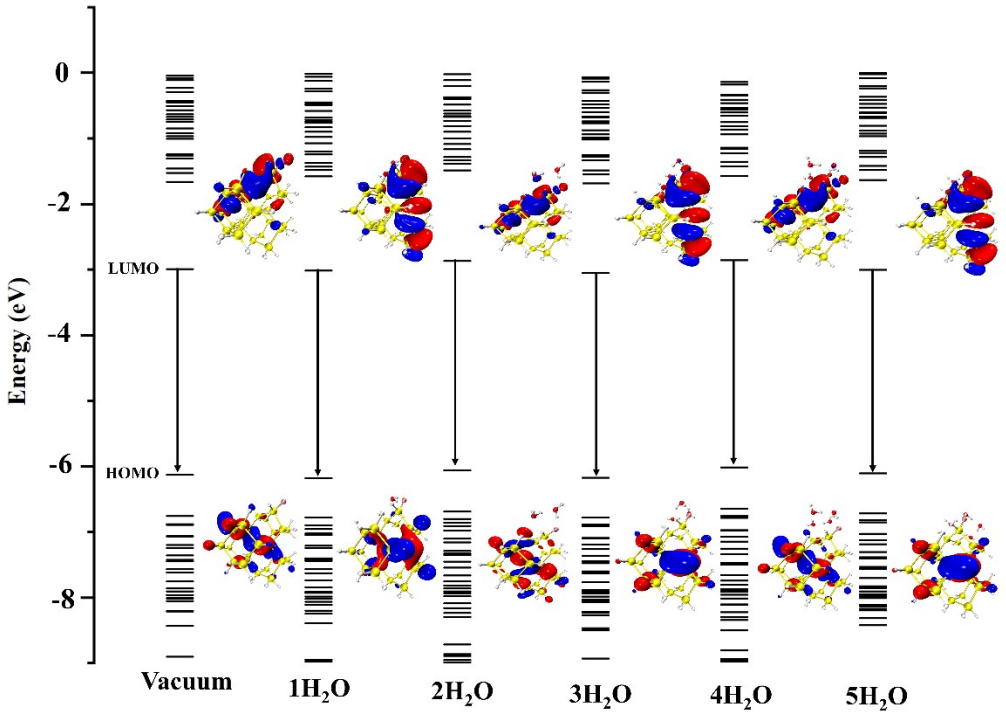

Figure S3b. Electronic transition orbits in excited states for Si-F in vacuum and the presence of one to five water molecules. Wave function isosurfaces are controlled at the same isovalue. The positive and negative phase parts of the orbital wave function are presented in red and blue, respectively. The thick arrows indicate electronic transitions of the excited state. The Si QDs ($Si_{29}H_{36}$) are presented in yellow. The oxygen and hydrogen atoms are shown in red, and white, respectively.

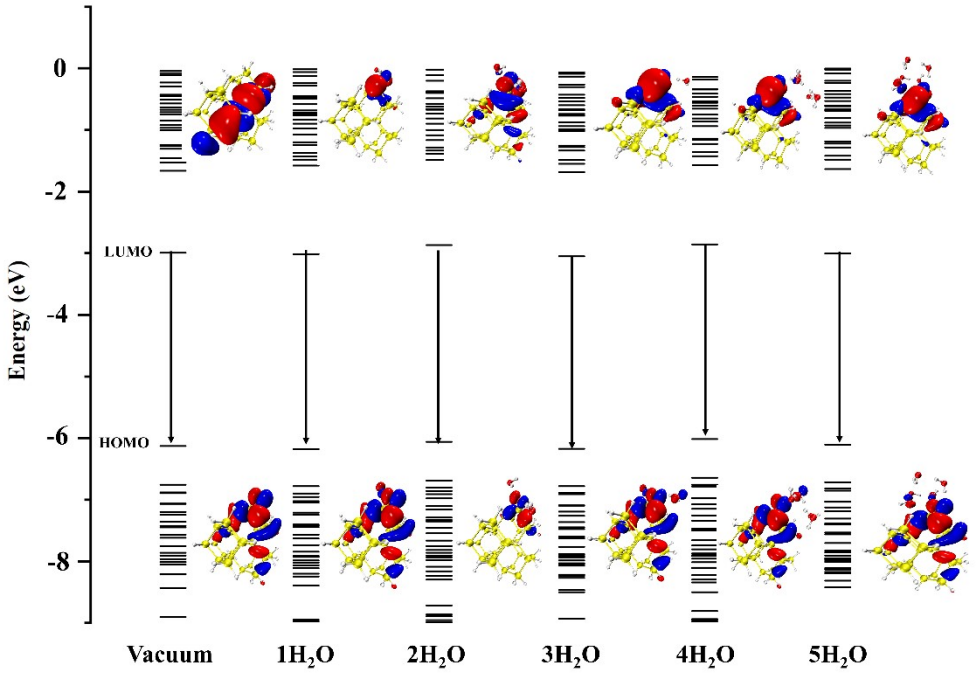

Figure S3c. Electronic transition orbits in excited states for Si-Si=O in vacuum and the presence of one to five water molecules. Wave function isosurfaces are controlled at the same isovalue. The positive and negative phase parts of the orbital wave function are presented in red and blue, respectively. The thick arrows indicate electronic transitions of the excited state. The Si QDs ($Si_{29}H_{36}$) are presented in yellow. The oxygen and hydrogen atoms are shown in red, and white, respectively.

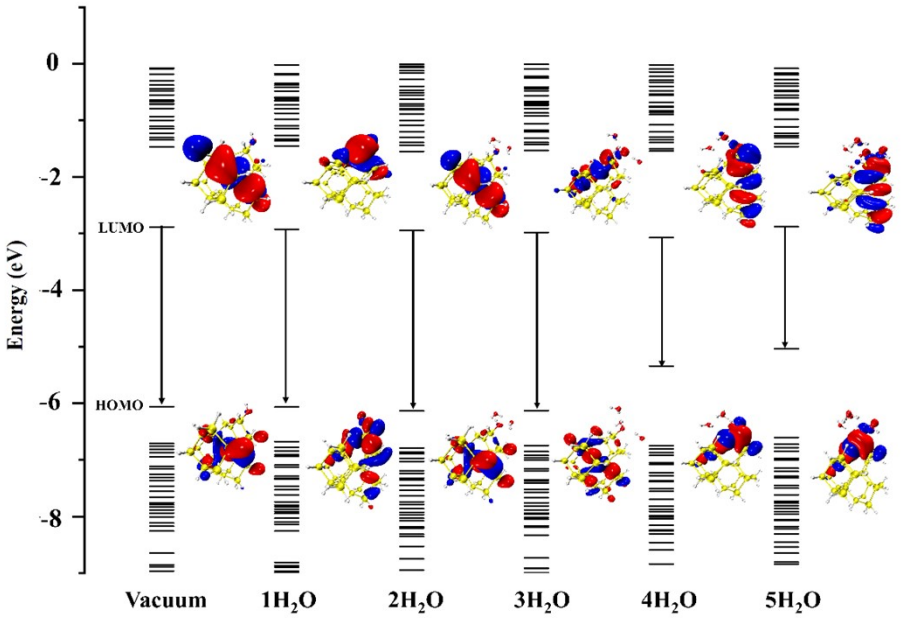

Figure S3d. Electronic transition orbits in excited states for Si-OH in vacuum and the presence of one to five water molecules. Wave function isosurfaces are controlled at the same isovalue. The positive and negative phase parts of the orbital wave function are presented in red and blue, respectively. The thick arrows indicate electronic transitions of the excited state. The Si QDs ($Si_{29}H_{36}$) are presented in yellow. The oxygen and hydrogen atoms are shown in red, and white, respectively.

The electrons in the lowest unoccupied molecular orbital (LUMO) of Si-H are linearly distributed in a vacuum or humid environment. The shape of electrons in the highest occupied molecules orbital (HOMO) with the distribution of its positive and negative phases is changed. Compared with LUMO orbitals, the positive and negative phase distribution of HOMO orbitals is more dispersed. The energy gap between LUMO and HOMO of Si-H under vacuum or humid environment is around 3.0 eV. The LUMO of Si-F is concentrated around hydroxyl groups and linearly distributed in vacuum or humid environment, whereas the HOMO distribution of Si-F is far from the F functional group. Compared to vacuum, the addition of water molecules makes the energies of the LUMO and HOMO of Si-F a little different. However, the energy gap between LUMO and HOMO of Si-F under vacuum or humid environment is also around 3.0 eV. The LUMO and HOMO of Si-Si=O are all concentrated around silicon-oxygen double bond groups in vacuum and in the presence of water molecules. The LUMO and HOMO of Si-Si=O are more localized near the functional group than those of Si-F. The energy gap between LUMO and HOMO of Si-Si=O is around 3.0 eV, whether in vacuum or water environment. This implies that the water environment has little effect on the LUMO and HOMO distributions of Si-Si=O and Si-F. In addition, the LUMO and HOMO of Si-OH are not concentrated around hydroxyl groups in vacuum and 2 or 3 water molecules environment, whereas the LUMO and HOMO of Si-OH are concentrated around hydroxyl groups in presence of 1 or 4 or 5 water molecules. The shape of HOMO with the distribution of its positive and negative phases is changed, compared with LUMO. The energy gap between LUMO and HOMO of Si-OH under vacuum or 1-3 water molecules environment is also around 3.0 eV. However, the energy gap between LUMO and HOMO of Si-OH is reduced to 2.4 eV. This implies that for hydroxyl-modified surfaces, the fluorescence can be tuned by water molecules.

Section 6. Root mean square displacement (RMSD) of silicon-silicon bond length between ground state and excited state

Definition of RMSD:

$$RMSD = \sqrt{\frac{1}{N}\sum_{i}^{natom}\left[\left(x_i - x_i^{'}\right)^2 + \left(y_i - y_i^{'}\right)^2 + \left(z_i - z_i^{'}\right)^2\right]}$$

where *i* circulates all atoms, x_i and x_i' are the x-coordinates of the *i*th atom in the first structure and the second structure, respectively, and y, z are similar. Superposition is performed before calculating the RMSD between the two structures.

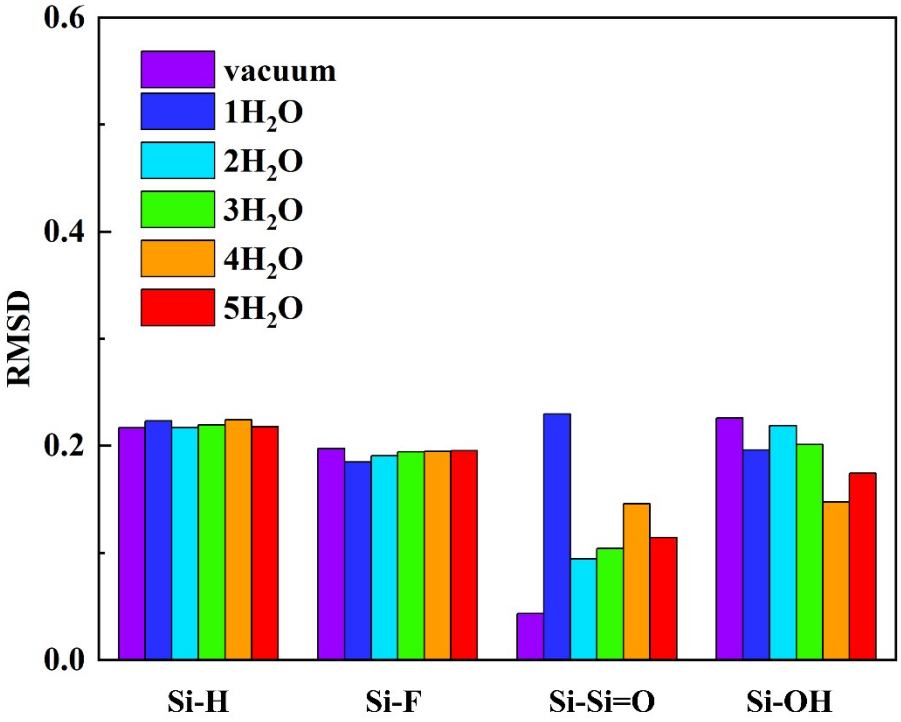

Figure S4. RMSD of silicon-silicon bond length between the ground state and excited state. The RMSD data from left to right are Si QDs passivated with H (Si-H), F (Si-F), Si=O (Si-Si=O), and OH (Si-OH), under vacuum and the environment of one to five water molecules.

The RMSD calculation to measure the change of the excited state structure relative to the ground state was performed. It is appropriate and convenient to measure the extent of change in the overall structure. As shown in **Figure S4,** the values of all RMSD are small, which indicates that the excited state structure is not much different from that of the ground state. For Si-H and Si-F, the calculated RMSD shows that the Si-Si bond length of the whole system in the excited state does not change much from the ground state, whether in vacuum or water environment. The RMSD of Si-Si=O is less than 0.1 Å under vacuum, and its RMSD increases (about 0.1-0.2 Å) when water molecules are adsorbed. The RMSD of Si-OH is about 0.2 Å in vacuum or humid environment.

Section 7. Excited and ground-state silicon-silicon bond length distribution of silicon quantum dots

In order to know more clearly the effect of structural changes on fluorescence, the bond lengths of Si-Si bonds of all structures were calculated and counted. The bond length distribution of Si-Si bonds in each system is drawn, and the comparison of the positions with the largest changes in the system

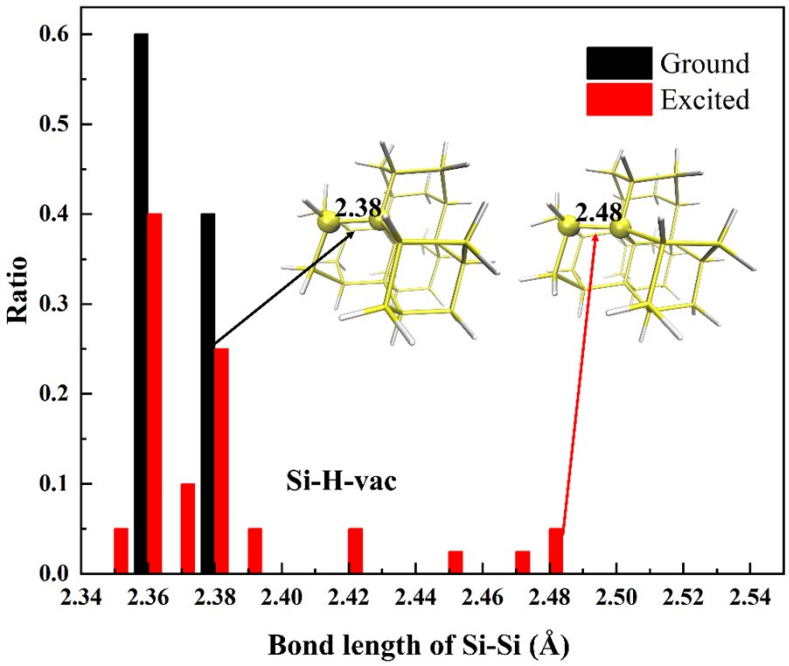

Figure S5a. The distribution of Si-Si bond lengths of Si-H-vac in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ under vacuum are briefly expressed as Si-H-vac. The insets depict the geometric structures of Si-H-vac in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

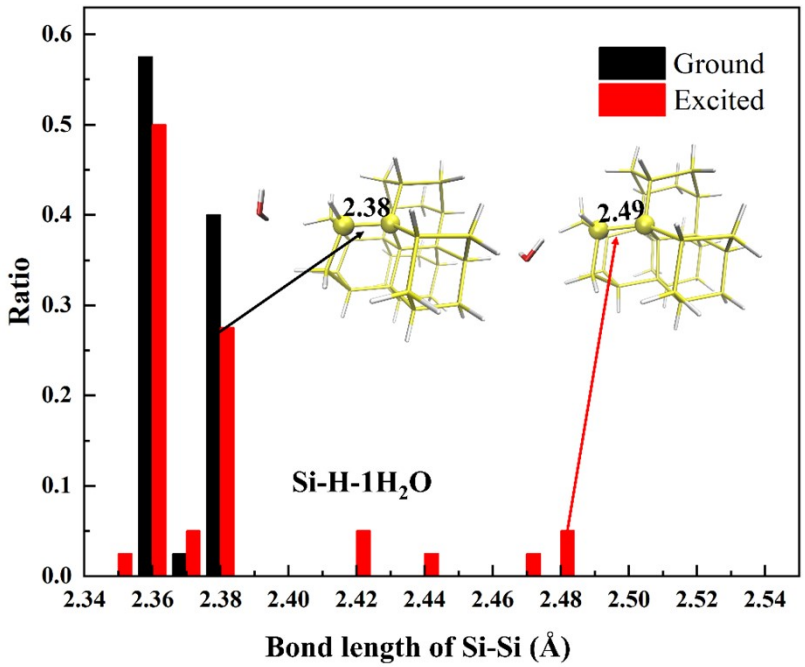

Figure S5b. The distribution of Si-Si bond lengths of Si-H-1H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ with one water molecule is briefly expressed as Si-H-1H_2O. The insets depict the geometric structures of Si-H-1H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

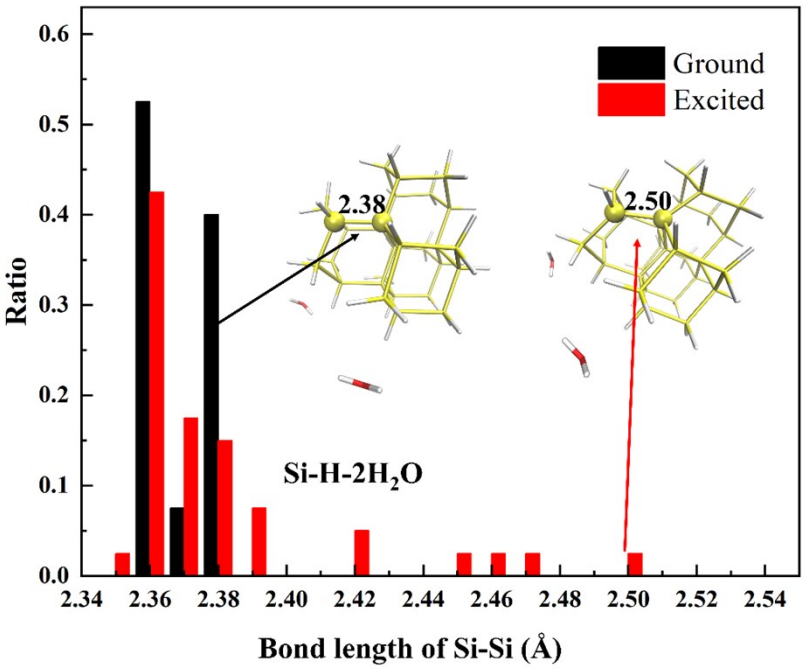

Figure S5c. The distribution of Si-Si bond lengths of Si-H-2H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ with two water molecules is briefly expressed as Si-H-2H_2O. The insets depict the geometric structures of Si-H-2H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

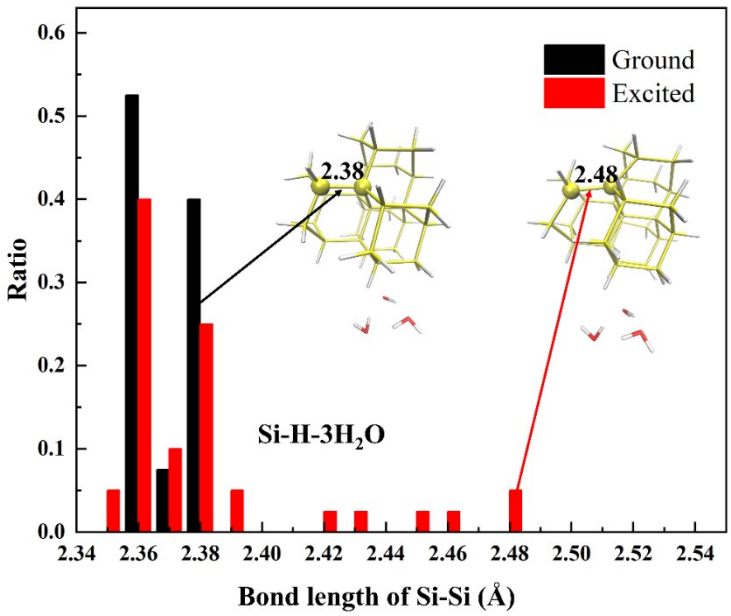

Figure S5d. The distribution of Si-Si bond lengths of Si-H-3H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ with three water molecules is briefly expressed as Si-H-3H_2O. The insets depict the geometric structures of Si-H-3H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

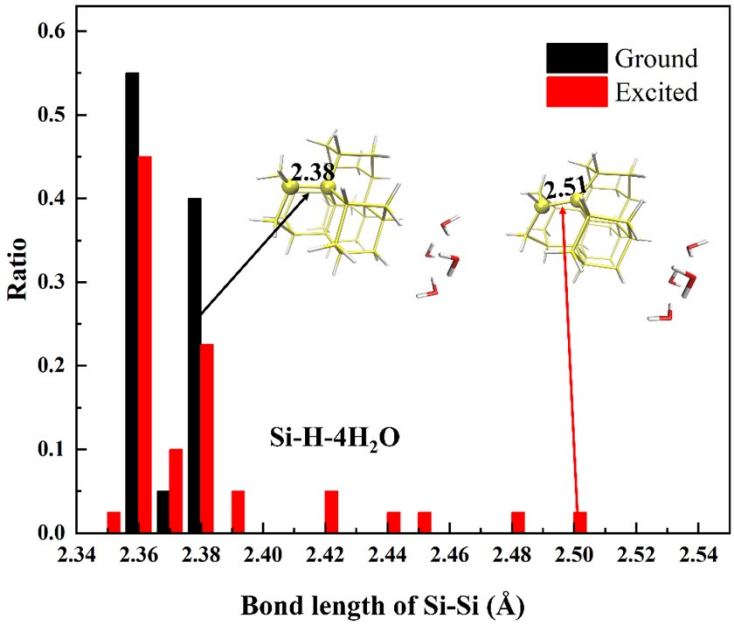

Figure S5e. The distribution of Si-Si bond lengths of Si-H-4H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ with four water molecules is briefly expressed as Si-H-4H_2O. The insets depict the geometric structures of Si-H-4H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

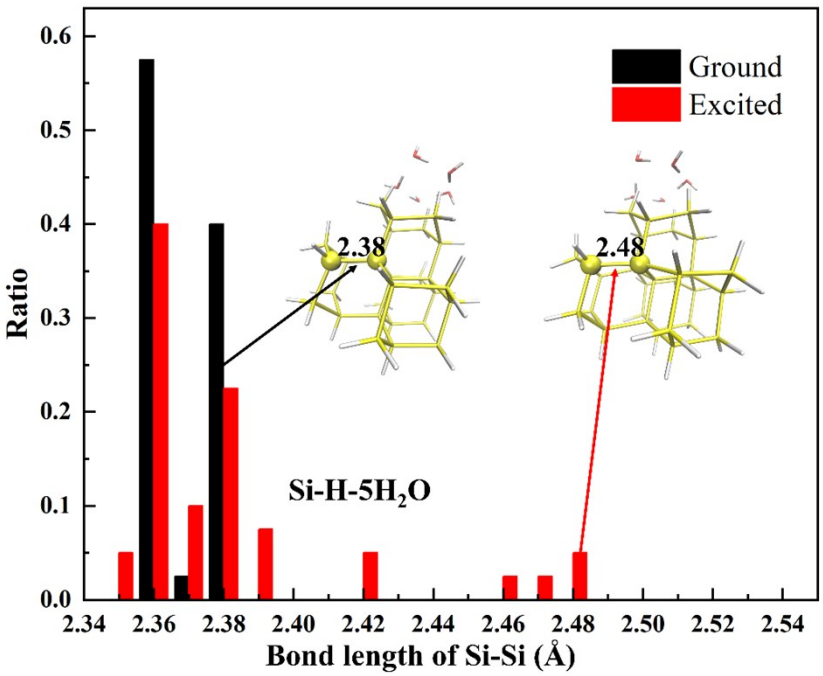

Figure S5f. The distribution of Si-Si bond lengths of Si-H-5H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{36}$ with five water molecules is briefly expressed as Si-H-5H_2O. The insets depict the geometric structures of Si-H-5H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

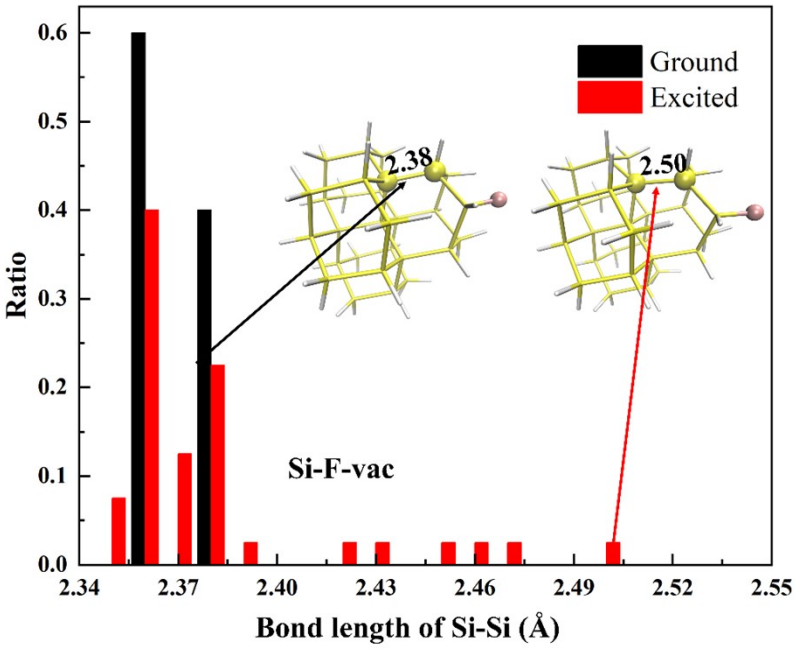

Figure S6a. The distribution of Si-Si bond lengths of Si-F-vac in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ under vacuum are briefly expressed as Si-F-vac. The insets depict the geometric structures of Si-F-vac in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

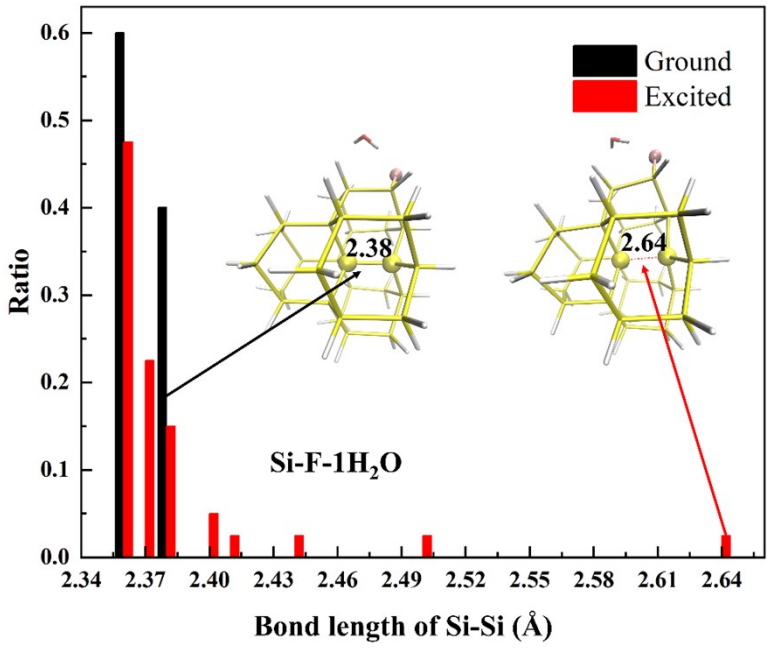

Figure S6b. The distribution of Si-Si bond lengths of Si-F-1H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ with one water molecule is briefly expressed as Si-F-1H_2O. The insets depict the geometric structures of Si-F-1H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

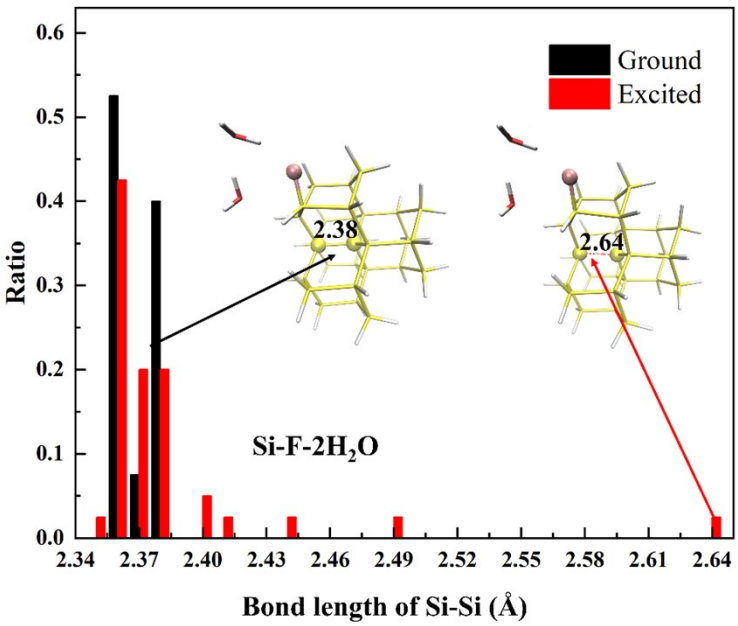

Figure S6c. The distribution of Si-Si bond lengths of Si-F-2H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ with two water molecules is briefly expressed as Si-F-2H_2O. The insets depict the geometric structures of Si-F-2H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

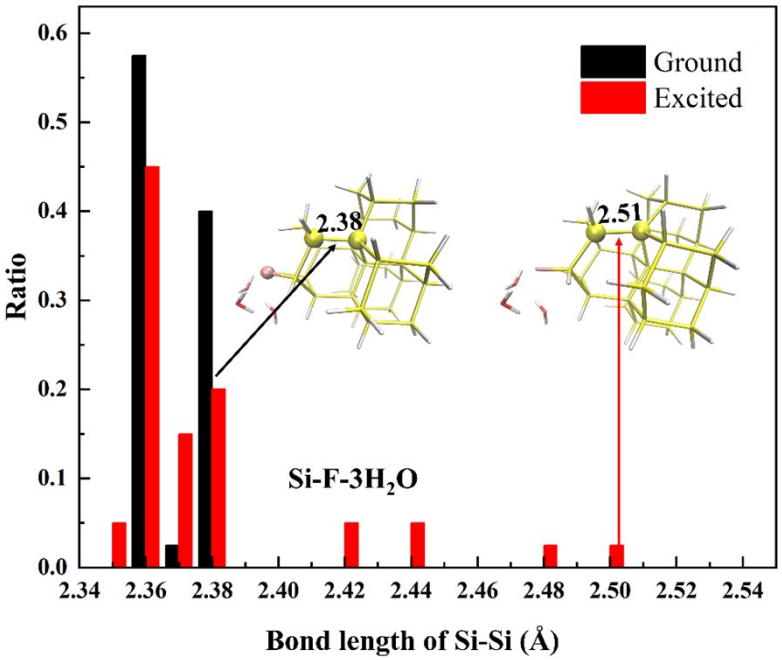

Figure S6d. The distribution of Si-Si bond lengths of Si-F-3H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ with three water molecules is briefly expressed as Si-F-3H_2O. The insets depict the geometric structures of Si-F-3H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

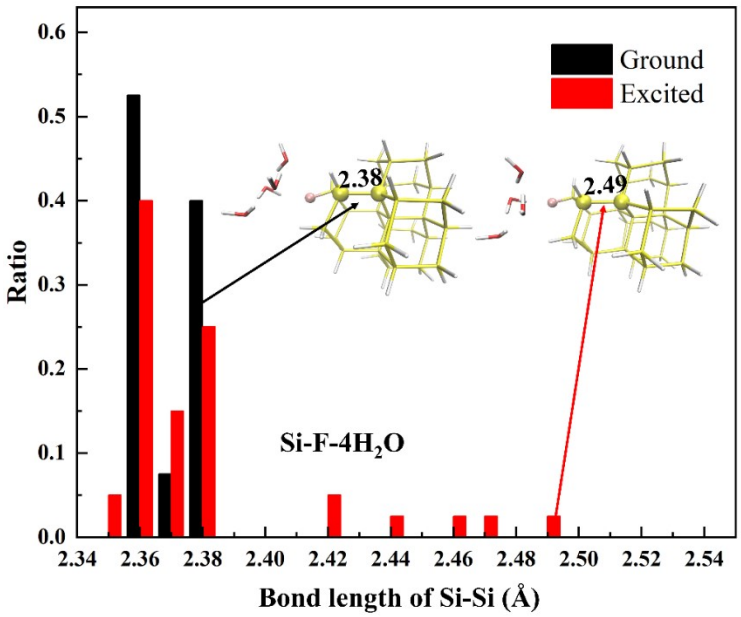

Figure S6e. The distribution of Si-Si bond lengths of Si-F-4H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ with four water molecules is briefly expressed as Si-F-4H_2O. The insets depict the geometric structures of Si-F-4H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

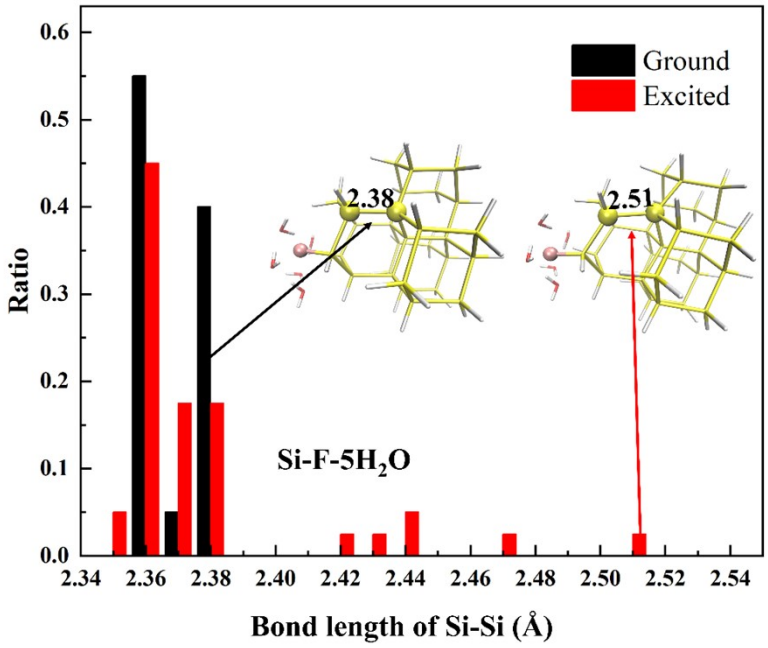

Figure S6f. The distribution of Si-Si bond lengths of Si-F-5H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}F$ with five water molecules is briefly expressed as Si-F-1H_2O. The insets depict the geometric structures of Si-F-1H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

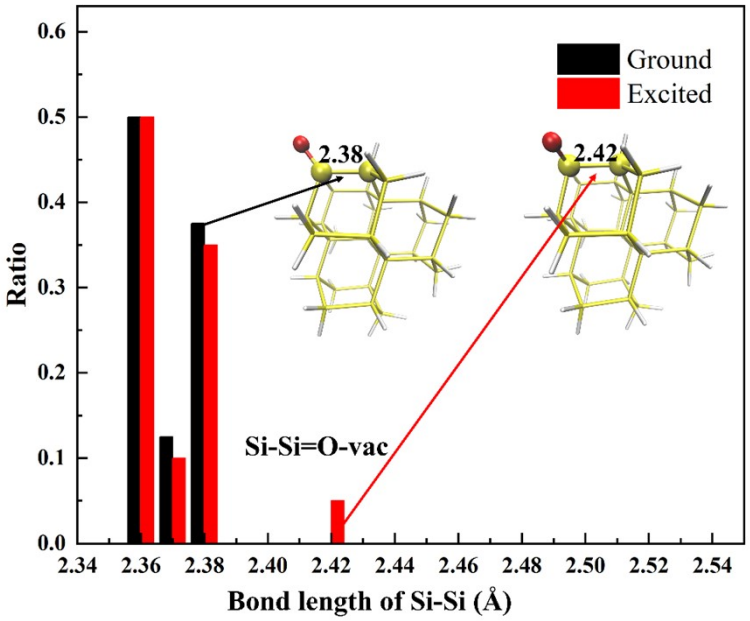

Figure S7a. The distribution of Si-Si bond lengths of Si-Si=O-vac in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si{=}O$ under vacuum is briefly expressed as Si-Si=O-vac. The insets depict the geometric structures of Si-Si=O-vac in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

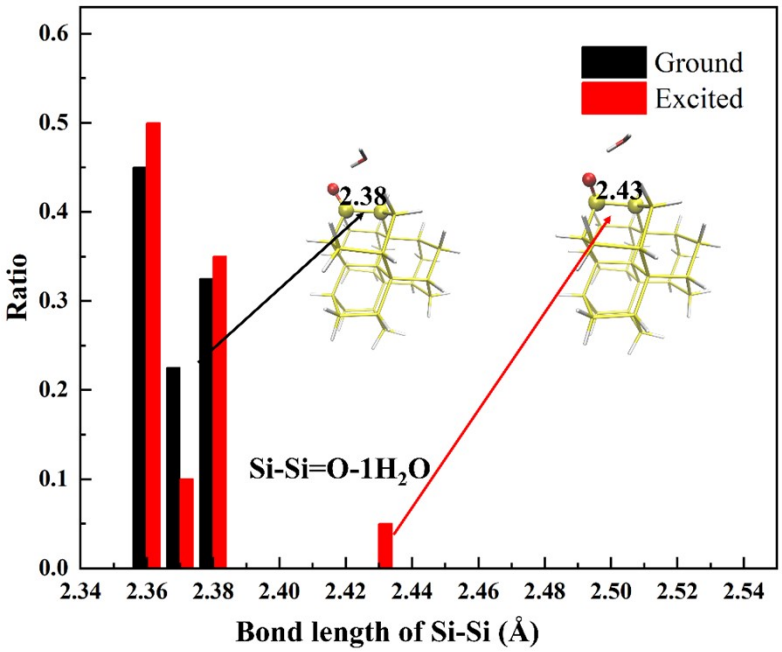

Figure S7b. The distribution of Si-Si bond lengths of Si-Si=O-1H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si$=O with one water molecule is briefly expressed as Si-Si=O-1H_2O. The insets depict the geometric structures of Si-Si=O-1H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

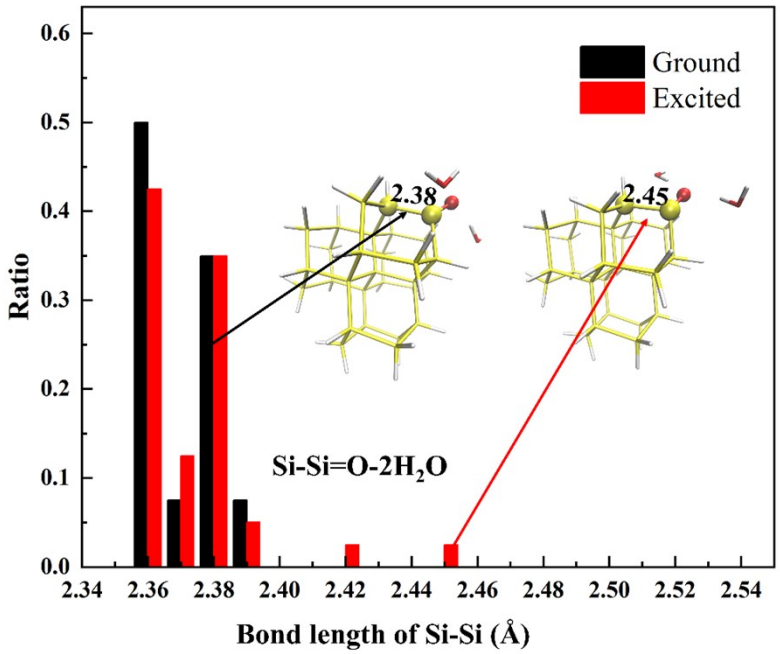

Figure S7c. The distribution of Si-Si bond lengths of Si-Si=O-2H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si$=O with two water molecule molecules is briefly expressed as Si-Si=O-2H_2O. The insets depict the geometric structures of Si-Si=O-2H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

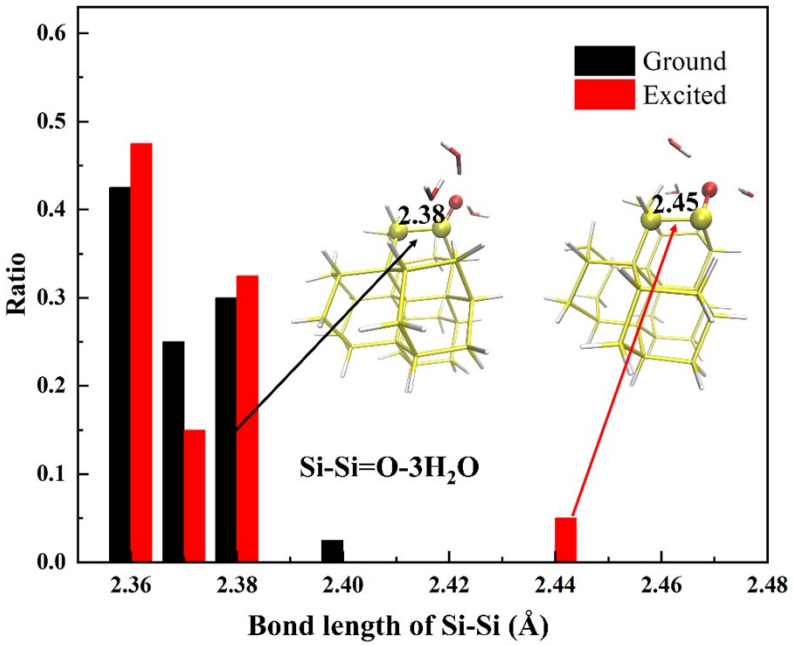

Figure S7d. The distribution of Si-Si bond lengths of Si-Si=O-3H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si$=O with three water molecules is briefly expressed as Si-Si=O-3H_2O. The insets depict the geometric structures of Si-Si=O-3H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

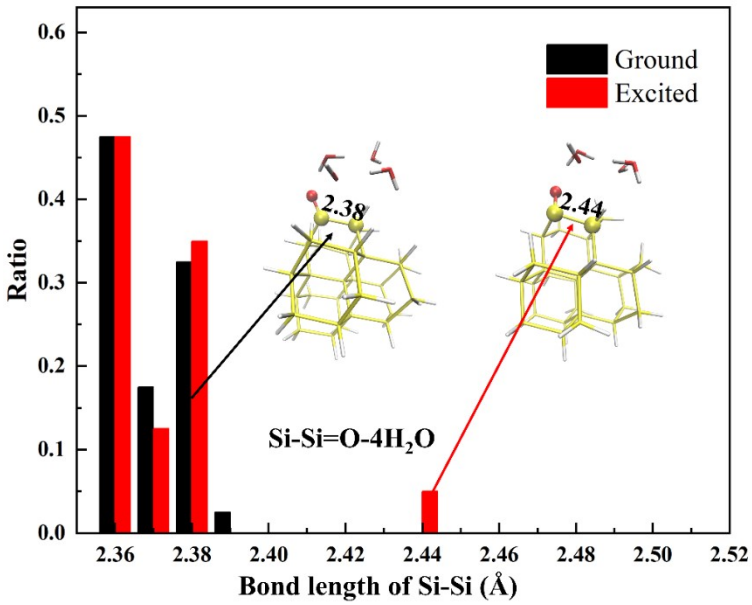

Figure S7e. The distribution of Si-Si bond lengths of Si-Si=O-4H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si$=O with four water molecules is briefly expressed as Si-Si=O-4H_2O. The insets depict the geometric structures of Si-Si=O-4H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

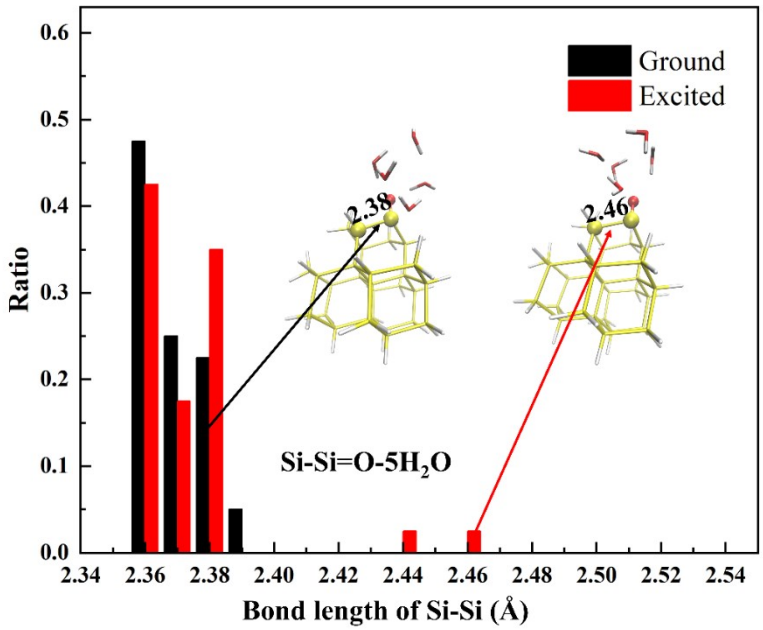

Figure S7f. The distribution of Si-Si bond lengths of Si-Si=O-5H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{34}Si$=O with five water molecules is briefly expressed as Si-Si=O-5H_2O. The insets depict the geometric structures of Si-Si=O-5H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

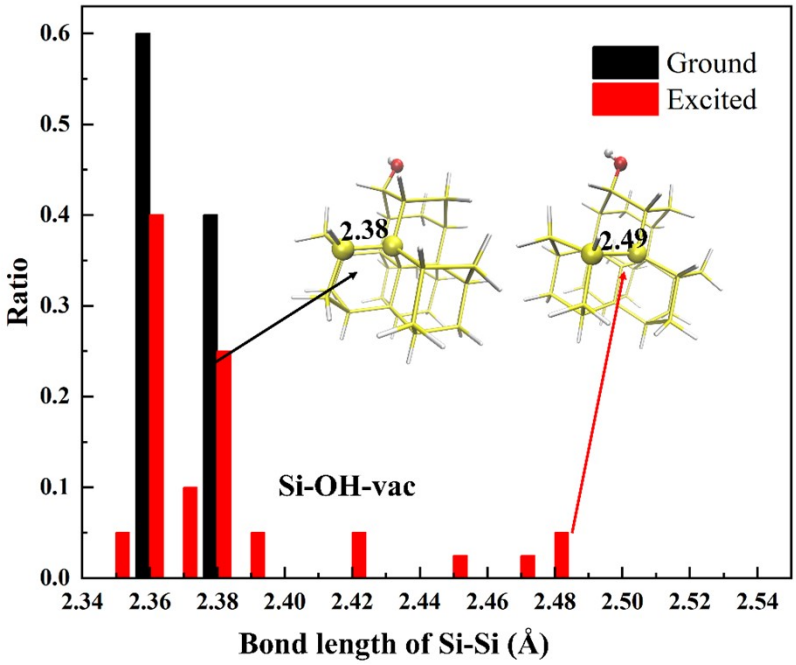

Figure S8a. The distribution of Si-Si bond lengths of Si-OH-vac in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ under vacuum is briefly expressed as Si-OH-vac. The insets depict the geometric structures of Si-OH-vac in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

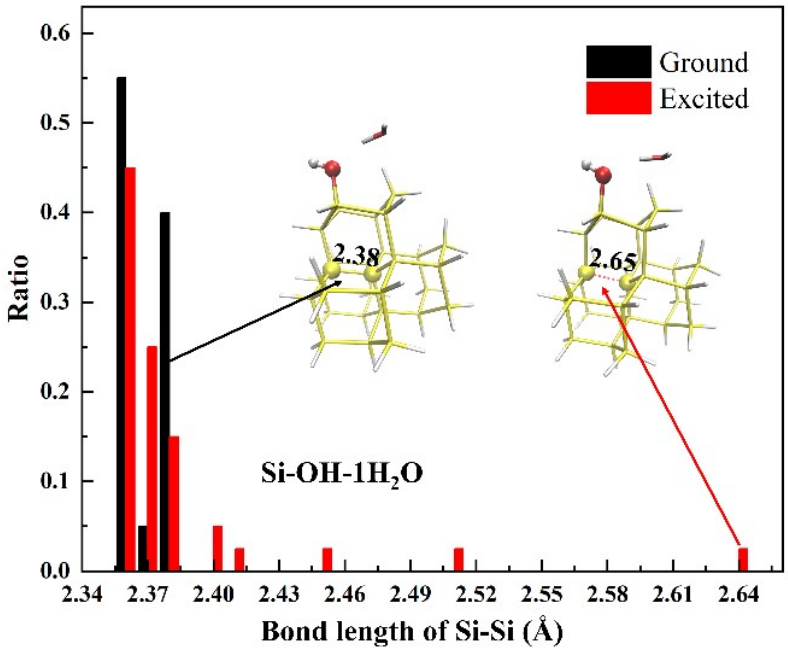

Figure S8b. The distribution of Si-Si bond lengths of Si-OH-1H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ with one water molecule is briefly expressed as Si-OH-1H_2O. The insets depict the geometric structures of Si-OH-1H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

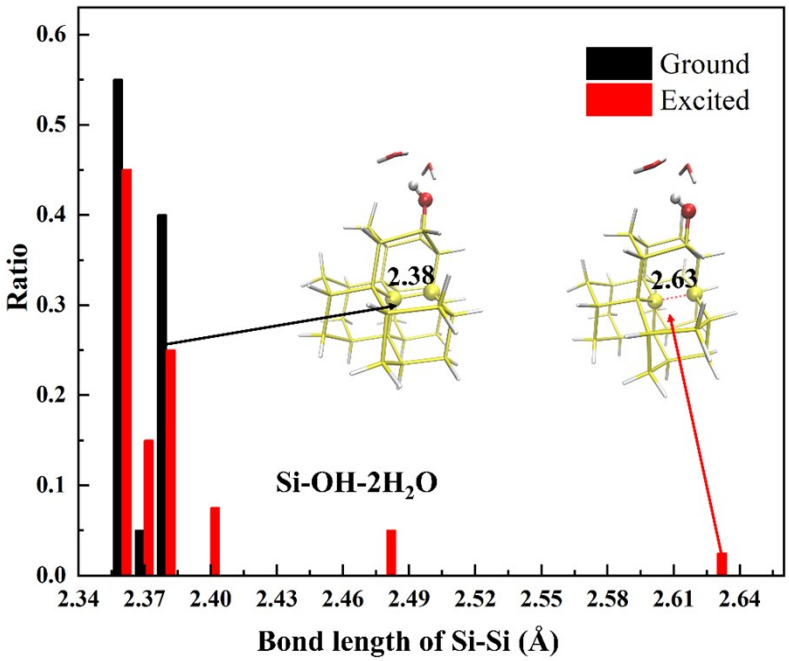

Figure S8c. The distribution of Si-Si bond lengths of Si-OH-2H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ with two water molecules is briefly expressed as Si-OH-2H_2O. The insets depict the geometric structures of Si-OH-2H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

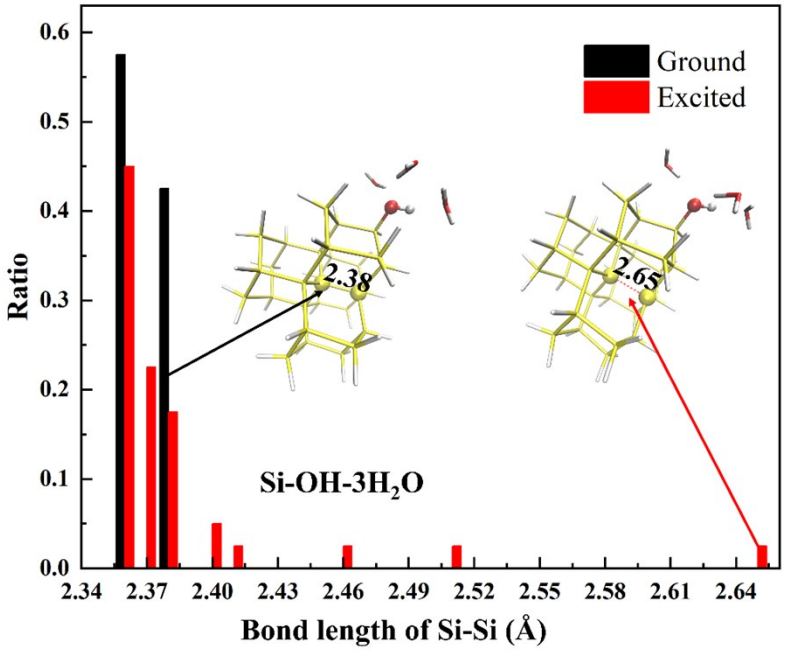

Figure S8d. The distribution of Si-Si bond lengths of Si-OH-3H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ with three water molecules is briefly expressed as Si-OH-3H_2O. The insets depict the geometric structures of Si-OH-3H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

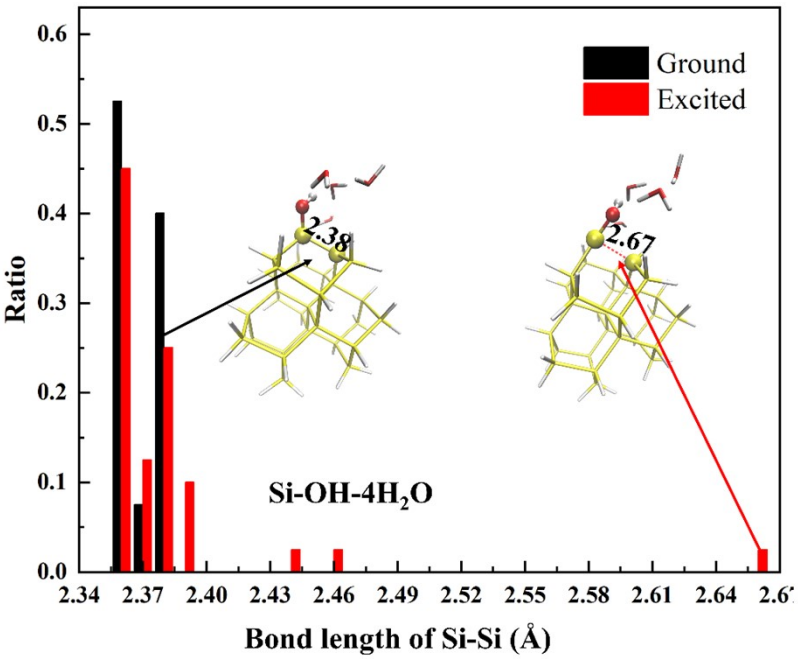

Figure S8e. The distribution of Si-Si bond lengths of Si-OH-4H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ with four water molecules is briefly expressed as Si-OH-4H_2O. The insets depict the geometric structures of Si-OH-4H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

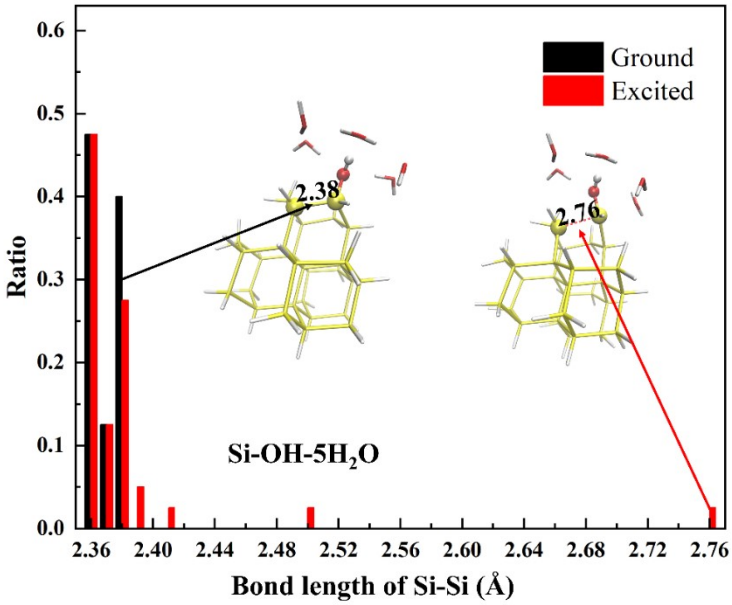

Figure S8f. The distribution of Si-Si bond lengths of Si-OH-5H_2O in the ground state (black histogram) and relaxed excited state (red histogram). The $Si_{29}H_{35}OH$ with five water molecules is briefly expressed as Si-OH-5H_2O. The insets depict the geometric structures of Si-OH-5H_2O in the ground state and excited state. The line with the arrow displays the largest stretched bond. Silicon, oxygen, and hydrogen atoms are colored in yellow, red, and white, respectively.

According to the Si-Si bond length distribution of Si-H, the major Si-Si bonds have a length of ~2.35 Å either in the ground state or in the excited state whether in a vacuum or in an aqueous environment. The largest Si-Si bond of Si-H in vacuum and 1-5 in water environment is 2.48 Å, 2.49 Å, 2.50 Å, 2.48 Å, 2.51 Å, 2.48 Å, in the excited state, respectively. The corresponding ground state silicon-silicon bond lengths are all 2.38 Å. As for the Si-Si bond length distribution of Si-F, the bond length of the Si-Si bond is mainly 2.35 Å in the ground state and excited state. The largest Si-Si bond length of Si-F under vacuum is 2.50 Å in the excited state, which compares with a corresponding bond length of 2.38 Å in the ground state. According to Figure S6b and Figure S6b, the maximum bond length of Si-F with one or two water molecules in the excited state is 2.64 Å, which is increased compared to that in vacuum (2.50 Å). Additionally, for Si-F in the excited state, the largest Si-Si bonds are at the cluster edges in vacuum, whereas the largest Si-Si bonds are at the cluster center in the presence of one or two water molecules. The largest Si-Si bonds of Si-F in four and five waters environment are 2.51 Å and 2.49 Å, respectively, which are at the cluster edges. As for the Si-Si=O, the major Si-Si bonds have a length of ~2.35 Å either in the ground state or in the excited state whether in a vacuum or in an aqueous environment. The largest Si-Si bonds of Si-Si=O in the excited state is 2.42 Å ~2.45 Å in vacuum or water environment, which is near the silicon-oxygen double bond functional group. The major Si-Si bonds of Si-OH have a length of ~2.35 Å either in the ground state or in the excited state whether in a vacuum or in an aqueous environment. The largest Si-Si bonds of Si-OH in the excited state is 2.49 Å in vacuum, whereas that is 2.63 Å ~2.65 Å in 1~3 water environment. In addition, the largest Si-Si bond of Si-OH in the excited state is 2.67 Å and 2.76 Å in the presence of four and five water molecules, respectively, which are near the hydroxyl group. This suggests that interactions between water molecules and between water molecules and hydroxyl groups cause changes in the quantum dot structure itself.

Section 8. Dipoles of silicon clusters in the ground state

The dipole moment is the product of the distance between the positive and negative charge centers and the amount of charge in the charge center. It is a vector whose direction is specified from the positive center to the negative center, represented by the symbol μ, and the unit is *D* (Debye). The mathematical expression for the dipole moment is $\mu = q$d. Depending on the object of discussion, the dipole moment can refer to the bond dipole moment or the molecular dipole moment. Molecular dipole moments can be obtained by vector addition of bond dipole moments. The dipole moment measured experimentally can be used to judge the spatial configuration of the molecule.

Table S5. Dipoles of different systems in the ground state.

System	μ (*D*)	System	μ (*D*)
Si-H-gas	0	Si-OH-gas	1.3
Si-H-1H_2O	1.4	Si-OH-1H_2O	2.5
Si-H-2H_2O	3.1	Si-OH-2H_2O	2.3
S-H-3H_2O	3.0	Si-OH-3H_2O	3.8
Si-H-4H_2O	1.6	Si-OH-4H_2O	1.9
Si-H-5H_2O	5.5	Si-OH-5H_2O	3.5
Si-F-gas	1.4	Si-Si=O-gas	4.9
Si-F-1H_2O	2.0	Si-Si=O-1H_2O	4.6
Si-F-2H_2O	2.5	Si-Si=O-2H_2O	3.9
Si-F-3H_2O	2.9	Si-Si=O-3H_2O	3.4
Si-F-4H_2O	3.5	Si-Si=O-4H_2O	4.9
Si-F-5H_2O	0.6	Si-Si=O-5H_2O	5.0

Section 9. Electrostatic potential map

The following is the electrostatic potential diagram of Si QDs passivated with pure H (Si-H), Si QDs substituted with one F (Si-F), Si QDs substituted with one Si=O (Si-Si=O), Si QDs substituted with one OH (Si-OH) under vacuum, (a) the electrostatic potential diagram from the functional group side to the upper left corner, (b) from the functional group of view top view. The column diagram is the electrostatic potential map with the electron density of the same isosurface (0.001 a.u). The color scale is from -50 to ~ 50 kcal/(mol·e). The extremum sites of its electrostatic potential with the extremum magnitude on the corresponding functional groups are annotated alongside.

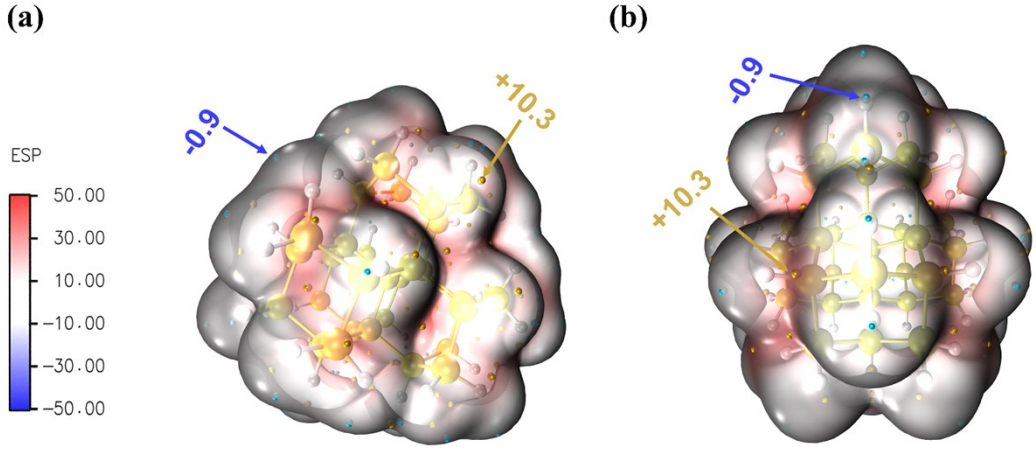

Figure S9a. The electrostatic potential diagrams of Si-H (a) The electrostatic potential map from the side of the replaced hydrogen atom to the upper left corner, and (b) Top view of the electrostatic potential diagram (looking down from the replaced hydrogen atom).

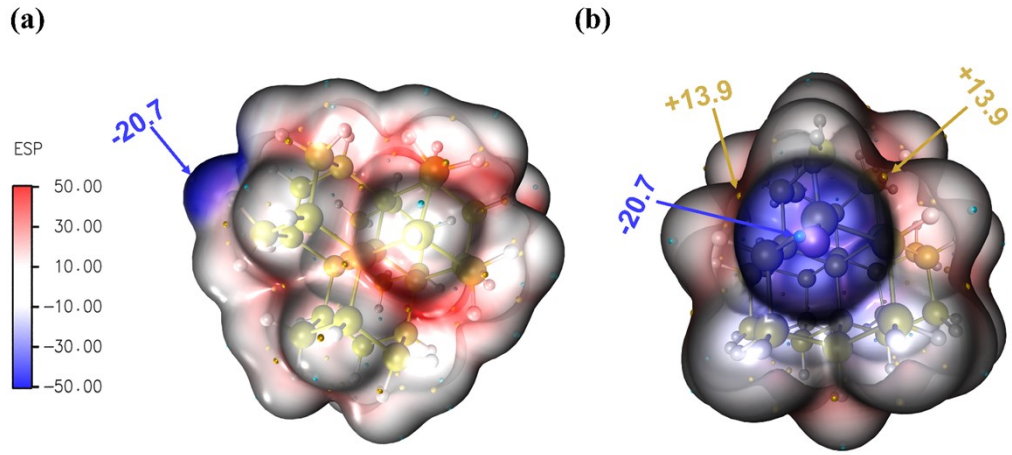

Figure S9b. Electrostatic potential diagram of Si-F (a) The electrostatic potential map from the side of the fluorine functional group to the upper left corner. (b) Top view of the electrostatic potential diagram (looking down from the fluorine functional group).

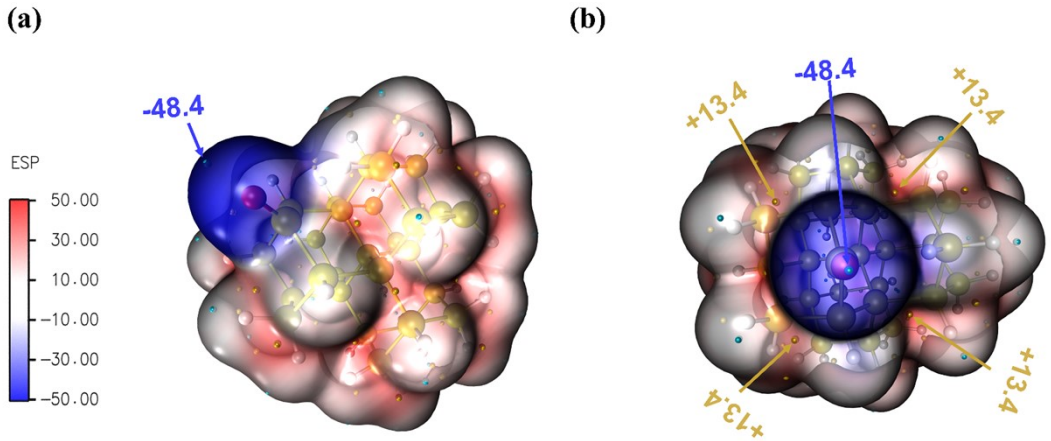

Figure S9c. Electrostatic potential diagram of Si-Si=O (a) The electrostatic potential map from the side of the silicon-oxygen double bond to the upper left corner. (b) Top view of the electrostatic potential diagram (looking down from the silicon-oxygen double bond).

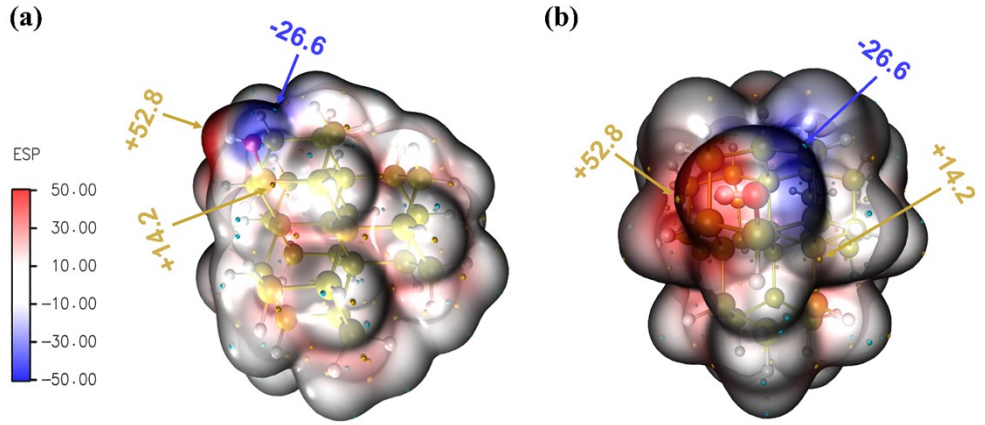

Figure S9d. Electrostatic potential diagram of Si-OH (a) The electrostatic potential map from the side of the hydroxyl functional group to the upper left corner. (b) Top view of the electrostatic potential diagram (looking down from the hydroxyl functional group).

Section 10. Dipole and adsorption energy of a single water molecule

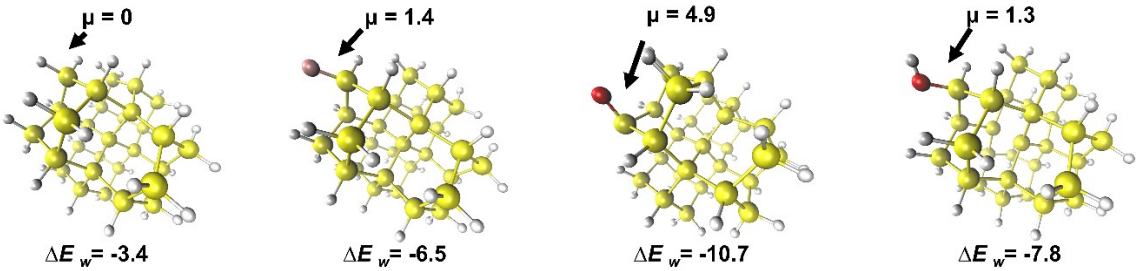

Figure S10. The **μ** represents the dipole of a single modified silicon quantum dot in the ground state. The ΔE_w is shown above and the unit is kcal/mol. The structure from left to right are Si QDs passivated with H (Si-H), Si QDs passivated with F (Si-F), Si QDs passivated with Si=O (Si-Si=O), and Si QDs passivated with OH (Si-OH). Silicon, oxygen, and hydrogen fluorine atoms are colored in yellow, red, and white, purple. respectively.

$$\Delta E_w = E(\text{cluster-surface}+H_2O) - E(\text{cluster-surface}) - E\ (H_2O)$$

The ΔE_w represents the decrease in system energy when a water molecule is adsorbed, E (cluster-surface+H_2O) represents the energy when a single water molecule is adsorbed on the surface of the silicon cluster (the water molecule is adsorbed on the surface close to the functional group when it is modified with a functional group), E(cluster-surface) represents the energy of the cluster, E (H_2O) represents the energy of one water molecule.

It can be seen from Figure S10 that the dipole of Si-H is approximately zero, and ΔE_w is -3.4 kcal/mol when a single water molecule is adsorbed on the cluster. The dipole of the Si-F system is larger than that of Si-H, which is 1.4 D. ΔE_w of Si-F is -6.5 kcal/mol, which is larger than that of Si-H. The dipole moment of the system reaches 4.9 D for the Si-Si=O, and ΔE_w of Si-Si=O is more than 10 kcal/mol (-10.7 kcal/mol). The dipole of the Si-OH system (1.3 D) is similar to that of the Si-F system (1.4 D), which implies that the dipole interactions of the Si-F and Si-OH structures themselves are similar in strength. ΔE_w of Si-OH is -7.8 kcal/mol, which is larger than that of Si-F.

Section 11. The test of the $Si_{29}H_{36}$ with water molecules away from the -OH functional group.

We also added some calculated data about the structures with water molecules away from the -OH functional group shown below (Figures S11a, S11b). We test the structures with four water molecules far from the $Si_{29}H_{36}$ with the OH group (Si-OH-4H2O_{far}).

It can be observed that the absorption spectra of Si-OH-4H2O_{far} show a single peak with the absorption wavelength of $S_0 \rightarrow S_1$ around 275nm (Figure S11a). The dual-band peaks can be observed in the PL spectra of Si-OH-4H2O_{far} as well, whereas the energy of Si-OH-4H2Ofar is higher than Si-OH surrounded by water molecules. It is reasonable for the water molecules to be absorbed around the functional groups.

Sum of electronic and thermal Energies of Si-OH-4H2O_{far} is about -8797.75 Hartree, and Sum of electronic and thermal Energies of the $Si_{29}H_{36}$ with -OH group surrounded by water molecules is -8797.77 Hartree.

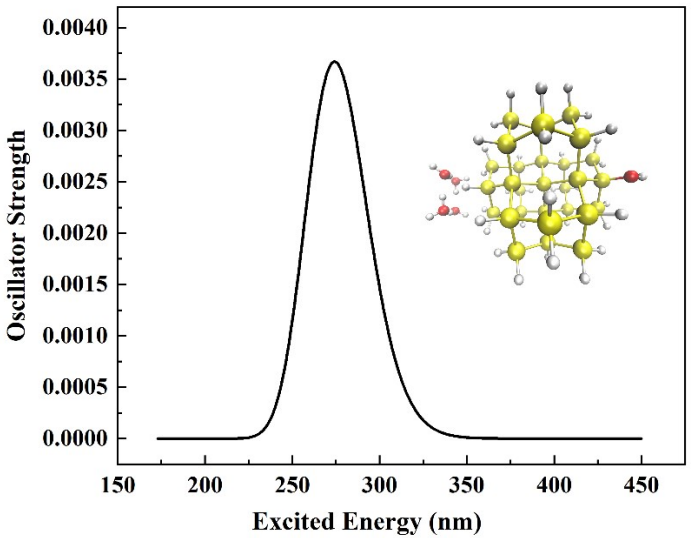

Figure S11a. The absorption spectra of Si-OH-4H_2O_{far} and the corresponding structures are inserted in the plots.

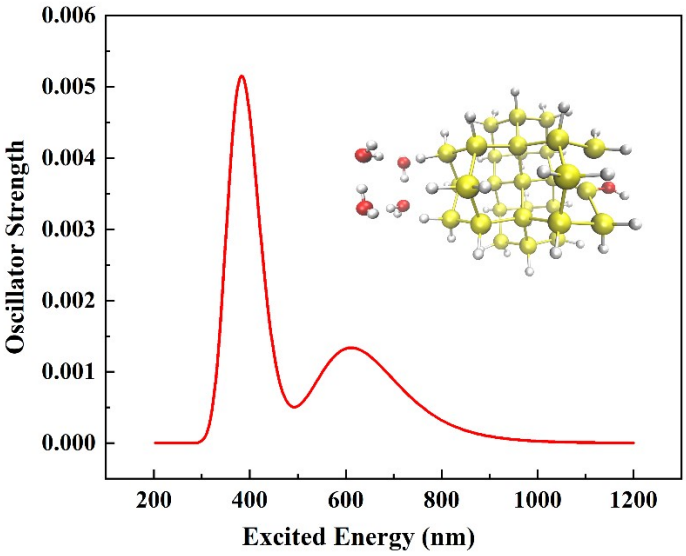

Figure S11b. The photoluminescence (PL) of Si-OH-4H_2O_{far} and the corresponding structures are inserted in the plots.

Section 12. The test of the impact of substituted hydrogen.

Since two hydrogen atoms are required for silicon-oxygen double bond substitution, we randomly chose silicon atoms with two replaceable hydrogen atoms for substitution in this study to circumvent the effect of different replacement hydrogens. Firstly, we optimized the $Si_{29}H_{36}$ cluster of pure hydrogen passivation to obtain a stable ground state structure. Then, a silicon atom containing two substitutable hydrogen atoms was selected for replacement. The coordinates of the silicon atom are marked with a yellow line (Table S6). The two hydrogen atoms with a blue line and a green line on this silicon atom were used to replace the silicon-oxygen double bond. Similarly, the hydrogen atom with a blue line was used to replace the hydroxyl or fluorine functional group. To avoid the bias caused by the random substitution of hydrogen, we chose three other hydrogens of the $Si_{29}H_{36}$ cluster to be replaced by hydroxyl groups in turn and then performed excitation and fluorescence calculations. The hydrogen atoms replaced with hydroxyl groups are marked in purple, red and gray, respectively. The photoluminescence and absorption spectra of these structures are almost indistinguishable as shown in Figures S12a and S12b.

Table S6. The Cartesian coordinates of $Si_{29}H_{36}$

Atom	x	y	z
Si	3.956615	2.361865	-0.32834
Si	0.993615	4.263785	-1.47239
Si	2.308278	2.374076	-2.02893
Si	1.5908	3.768009	2.147469
Si	2.930602	1.85697	1.745636
Si	1.045794	0.353523	-2.11854
Si	-2.19158	2.260693	-3.38003
Si	2.48516	-1.48857	-2.58681
Si	-0.64154	0.518819	-3.79511
Si	4.147377	-1.80953	-0.93042
Si	1.674005	-0.16858	1.695966
Si	-1.44788	1.835897	0.489971
Si	-0.15897	3.840693	0.552819
Si	3.106586	-2.00545	1.187964
Si	-0.00019	-0.00015	-7.3E-05
Si	-0.91703	1.199851	4.365407
Si	0.608892	-0.52088	3.799846
Si	-2.02519	-1.40011	-3.90878
Si	1.35196	-3.56813	-2.60387
Si	-1.272	-2.02133	-0.06753
Si	-4.39137	0.007294	-1.4339
Si	-3.10898	1.986206	-1.21383
Si	0.19142	-3.83885	-0.55721
Si	-2.93534	-1.831	-1.76521
Si	1.947565	-4.06369	1.015915
Si	-0.74966	-2.46055	3.83686
Si	-3.71227	-0.55876	2.692267
Si	-2.48071	1.462324	2.606099
Si	-2.30613	-2.35462	2.054791
H	4.823715	-3.10938	-1.21983

H	2.90597	-5.07421	0.476318
H	5.095611	1.458848	-0.63989
H	2.9619	2.593792	-3.35669
H	1.927586	5.403273	-1.22729
H	-3.3073	2.111231	-4.36172
H	0.015751	0.740192	-5.1208
H	3.138687	-1.26479	-3.91395
H	-3.16214	-1.0795	-4.82279
H	-3.38709	2.613116	2.910384
H	-1.06764	4.98891	0.860018
H	-4.01424	3.136644	-0.90488
H	-5.22402	0.147233	-2.66595
H	2.448133	4.971063	1.927297
H	-1.6718	0.750715	5.573438
H	1.65882	-0.62625	4.860521
H	3.978198	1.748763	2.808334
H	4.153663	-2.10886	2.25167
H	-1.52642	-2.43969	5.112428
H	-3.73076	-3.09754	-1.80557
H	-3.10182	-3.62084	2.010105
H	-0.60717	-5.10334	-0.59899
H	-4.10801	-0.78238	4.115028
H	0.044448	-3.71725	3.831135
H	1.477309	-4.56917	2.332376
H	4.509862	3.745709	-0.22976
H	5.196619	-0.75687	-0.9587
H	0.470183	-3.73114	-3.78953
H	-1.32472	-2.57923	-4.48226
H	-5.32686	-0.19938	-0.29719
H	-4.96608	-0.50114	1.895708
H	-0.2387	2.472994	4.724174
H	1.094812	3.83723	3.547152
H	0.084626	4.674902	-2.57444
H	-1.60621	3.611198	-3.58853
H	2.387226	-4.64219	-2.67766

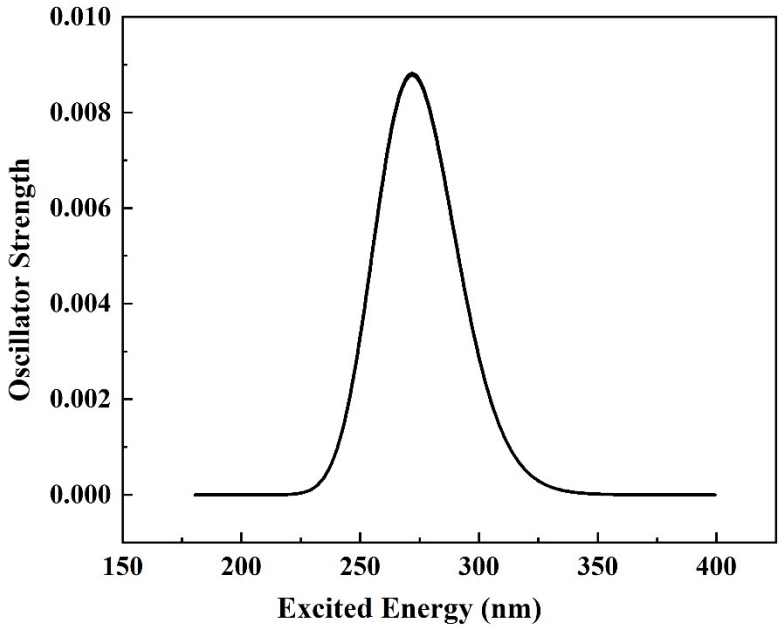

Figure S12a. The absorption spectra of the $Si_{29}H_{36}$ cluster replaced by hydroxyl groups in three different positions.

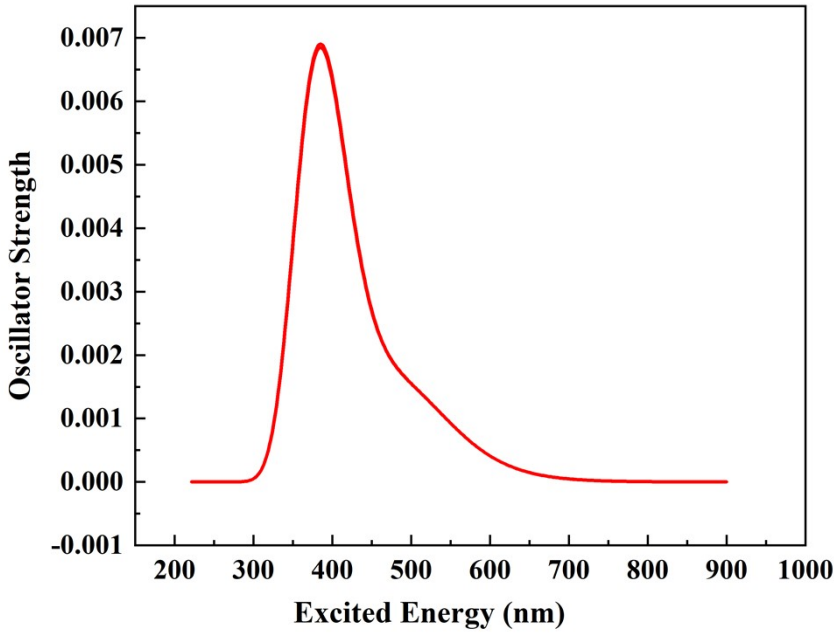

Figure S12b. The photoluminescence spectra of the $Si_{29}H_{36}$ cluster replaced by hydroxyl groups in three different positions.

Section 13. The data of the $Si_{29}H_{36}$ cluster with the B3LYP functional and 6-311G** basis set.

The photoluminescence and absorption spectra of $Si_{29}H_{36}$ with the substituent group of a hydrophilic hydroxyl (OH) surrounded by one or four water molecules were calculated with the B3LYP functional and 6-311G** basis set. We added the results in the manuscript as shown below:

The absorption wavelength of $S_0 \rightarrow S_1$ for the $Si_{29}H_{36}$ passivated by OH with one or four water molecules is around 275 nm (Figure S13a). The PL spectra of $Si_{29}H_{36}$ with OH surrounded by one water molecule indicate a single peak, whereas a dual-band peak appears in the case of four water molecules (Figure S13b). Therefore, the results of the larger basis set (6-311G**) are consistent with the basis set (6-31G*) in our manuscript.

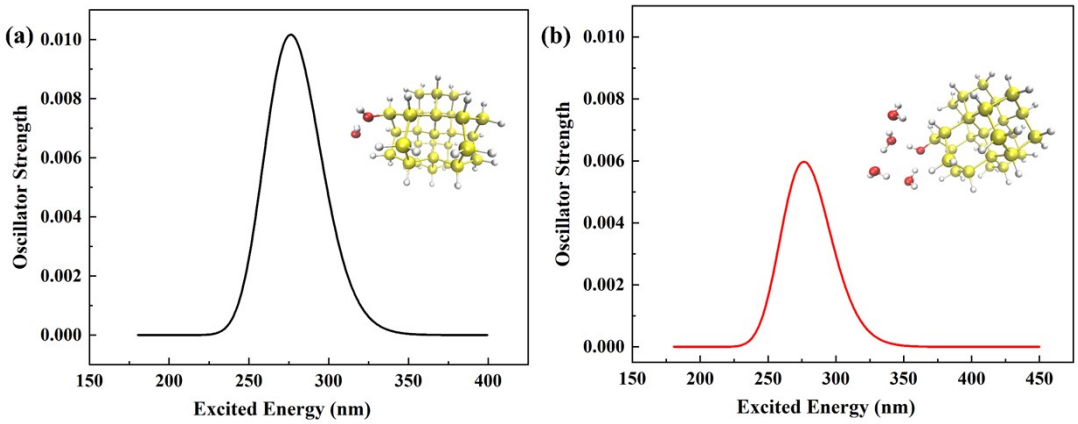

Figure S13a. The absorption spectra of $Si_{29}H_{36}$ with a hydrophilic hydroxyl (OH) surrounded by one water molecule (a) and four water molecules (b) and the corresponding structures are inserted in the plots.

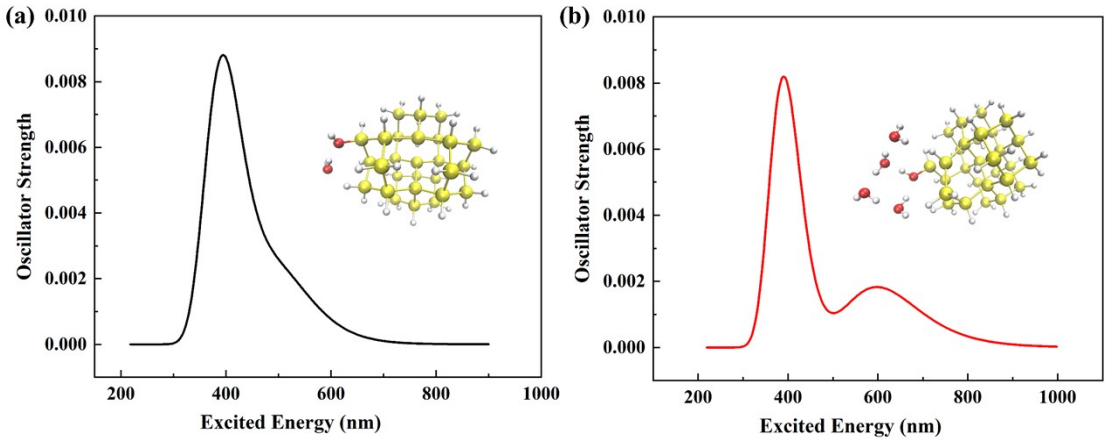

Figure S13b. The photoluminescence (PL) spectra of $Si_{29}H_{36}$ with a hydrophilic hydroxyl (OH) surrounded by one water molecule (a) and four water molecules (b) and the corresponding structures are inserted in the plots.

Section 14. The $Si_{29}H_{24}$ cluster with one terminal hydroxyl group.

To understand more clearly the effect of the configuration on the calculation results, the $Si_{29}H_{24}$ clusters with one terminating hydroxyl group in the two different substitution sites are constructed. The absorption and photoluminescence spectra are shown in **Figure S14a** and **Figure S14b**. The effect of water molecules is also considered in the $Si_{29}H_{24}$ cluster with a hydroxyl group. The absorption and photoluminescence spectra of the $Si_{29}H_{24}$ cluster with a hydroxyl group surrounded by one water molecule are shown in **Figure S14c** and **Figure S14d.**

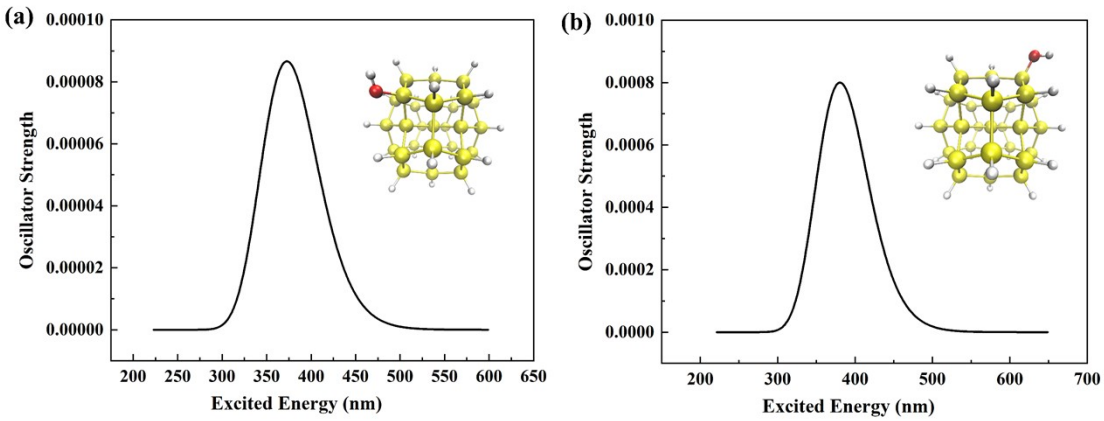

Figure S14a. The absorption spectra of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group and the corresponding structures are inserted in the plots.

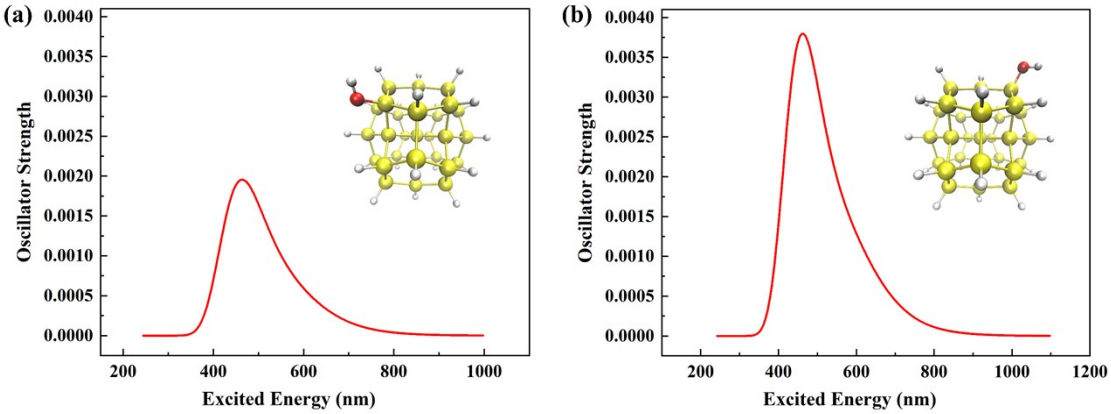

Figure S14b. The photoluminescence (PL) spectra of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group and the corresponding structures are inserted in the plots.

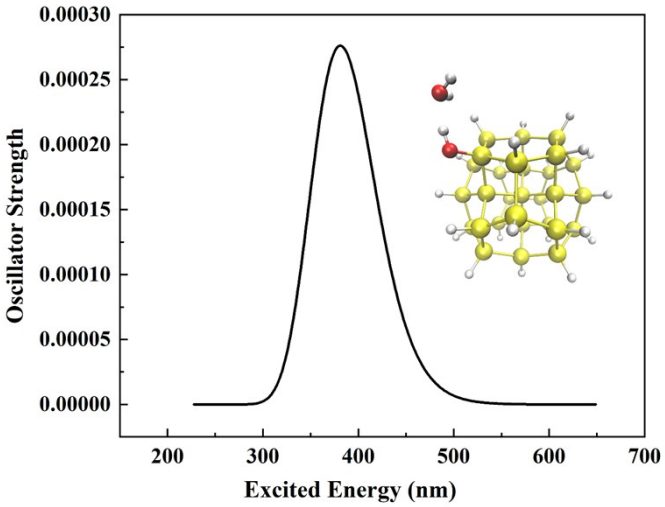

Figure S14c. The absorption spectra of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group surrounded by one water molecule and the corresponding structure is inserted in the plot.

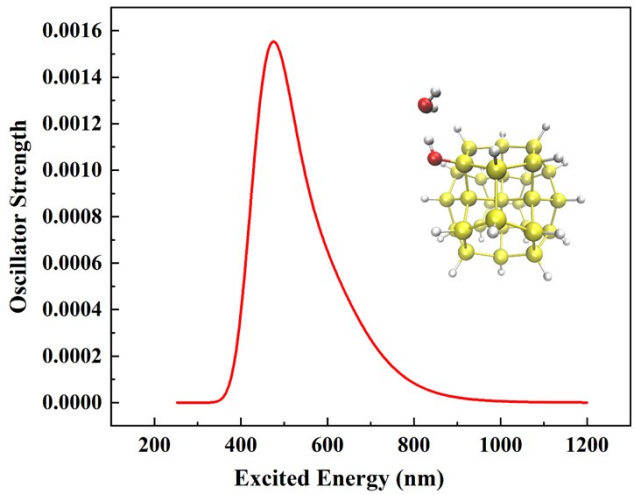

Figure S14d. The photoluminescence spectra of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group surrounded by one water molecule and the corresponding structure is inserted in the plot.

Table S7. Excitation wavelengths (EX) of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group in different substitution sites ($Si_{29}H_{24}$-A and $Si_{29}H_{24}$-B) and surrounded by a water molecule ($Si_{29}H_{24}$-H_2O).

System	EX in nm (eV)
$Si_{29}H_{24}$-A	375 (3.3)
$Si_{29}H_{24}$-B	381 (3.2)
$Si_{29}H_{24}$-H_2O	385 (3.2)

Table S8. Emission wavelengths (EM) of $Si_{29}H_{24}$ with a hydrophilic hydroxyl group in different substitution sites ($Si_{29}H_{24}$-A and $Si_{29}H_{24}$-B) and surrounded by a water molecule ($Si_{29}H_{24}$-H_2O).

System	EM in nm (eV)
$Si_{29}H_{24}$-A	566 (2.2)
$Si_{29}H_{24}$-B	577 (2.1)
$Si_{29}H_{24}$-H_2O	598 (2.1)

The cartesian coordinates of the $Si_{29}H_{24}$ cluster with one terminating hydroxyl group in the two different substitution sites ($Si_{29}H_{24}$-A and $Si_{29}H_{24}$-B) and surrounded by a water molecule ($Si_{29}H_{24}$-H_2O) are shown below.

$Si_{29}H_{24}$-A

Si	-0.67793100	-3.95242000	-0.93200300
Si	-2.19072800	-0.73096600	-3.36219000
Si	-2.33908800	-2.43642400	-1.70875100
Si	2.03562300	-1.57620300	-3.29331100
Si	1.46087800	-3.19062400	-1.64315100
Si	-2.10838700	-0.98331100	0.08276100
Si	-3.06745700	1.35789700	-2.27096000
Si	-2.33813100	-2.11802900	2.09105200
Si	-3.67484600	0.70727400	-0.05827100
Si	-0.67757800	-3.74262600	1.57515300
Si	1.75144700	-1.74456000	0.14451600
Si	0.37369700	1.20062200	-2.08246300
Si	0.10156700	-0.29832200	-3.82888700
Si	1.46218400	-2.87444500	2.14759300
Si	0.09512500	0.00786300	-0.00028800
Si	3.62046200	0.01805000	-2.16613800
Si	3.85646000	-0.77747500	0.06320300
Si	-3.06617100	1.71657700	2.01547900
Si	-2.18845700	-0.16190600	3.43844900
Si	0.37543600	1.52912700	1.85515100
Si	-0.35372000	4.09300800	-0.34165300
Si	-1.23047000	2.86898500	-2.18393900
Si	0.10436100	0.34054900	3.82606500
Si	-1.22898800	3.19171200	1.67857700
Si	2.03777000	-1.00969900	3.50742100
Si	3.62224000	0.37561400	2.13080000
Si	2.11093800	3.59689700	-0.30054600
Si	2.50176700	2.11701100	-2.12181500
Si	2.50374400	2.43891200	1.74070600
H	-0.94998900	-5.08039700	2.18810200
H	2.70113000	-1.39743700	4.79152600
H	-3.69833400	-3.05708600	-1.67827600
H	-2.99148000	-1.03260300	-4.58976600
H	-4.22025700	1.88980700	-3.06647100
H	-3.69732200	-2.73486700	2.16556900
H	-4.21882000	2.37331900	2.71169700
H	2.69246000	2.86668200	-3.40238300
H	0.26816300	0.42416100	-5.12832900
H	-1.08190800	3.62769900	-3.46495000
H	-0.56358800	5.56963200	-0.46509300
H	2.69824000	-2.17119200	-4.49585200
H	4.91342800	0.05522300	-2.91854300
H	4.89272300	-1.85281500	0.15193900
H	2.48494100	-4.27849600	-1.56437900
H	2.48616700	-3.96049300	2.24891800
H	4.91546500	0.53643700	2.86632300
H	-1.08117900	4.15324500	2.81523800
H	2.69527100	3.38989600	2.87964000
H	0.27275900	1.26810300	4.98784100
H	2.87832400	4.87716000	-0.40789400
H	-0.94986200	-5.37357100	-1.31392700
H	-2.98866200	-0.25557200	4.69943300
O	-5.21367400	0.00619400	0.00064100
H	-5.95274000	0.63038400	-0.05134400

$Si_{29}H_{24}$-B

Si	-0.32388700	-3.49662200	-2.19561900
Si	3.22299900	-2.44511900	0.01863500
Si	1.88298800	-2.64887100	-1.93590800
Si	-0.38160400	-3.54331000	2.11452000
Si	-1.35546300	-3.63940900	-0.05534000
Si	1.23646300	-0.42233500	-1.94723200
Si	4.04220600	-0.04862600	0.04012500
Si	-0.02904000	0.03645500	-3.83414500
Si	3.09681900	0.96309700	-1.88899300
Si	-1.58740900	-1.71982700	-3.44957900
Si	-2.07289600	-1.43586600	-0.04059700
Si	1.18859500	-0.46508400	1.96957000
Si	1.83102200	-2.69272900	1.92938100
Si	-3.27660000	-0.95001300	-1.95984800
Si	-0.12377500	-0.00518600	-0.00004300
Si	-1.67475600	-1.79218000	3.37254800
Si	-3.32630200	-0.99169700	1.85726600
Si	1.84947200	2.97608800	-2.10011000
Si	-0.22041800	2.36521900	-3.38788600
Si	-0.80433100	2.31417100	0.01733600
Si	1.79343700	2.92990900	2.21701200
Si	3.04750800	0.92320800	1.98052200
Si	-2.04124100	2.72474800	-1.89902900
Si	1.09416100	3.64360600	0.05621300
Si	-3.82156500	1.26833400	-1.29187700
Si	-3.85446700	1.24084300	1.22370100
Si	-0.30844200	2.29212600	3.43643800
Si	-0.12525800	-0.04585900	3.83310900
Si	-2.09084300	2.68285300	1.90945600
H	-2.14114000	-2.30241100	-4.71163500
H	-5.15344000	1.72180800	-1.80140300
H	2.72045900	-2.92369700	-3.14470900
H	4.40102100	-3.37121900	0.02692900
H	0.79419600	-0.21974800	-5.05675300
H	2.58915400	4.05625400	-2.82428100
H	0.66591800	-0.32956500	5.07093600
H	2.63542300	-2.99030700	3.15613000
H	3.84598500	0.61923400	3.21206300
H	2.51490400	3.99334600	2.98355500
H	-0.46080100	-4.84483400	2.84894800
H	-2.25810000	-2.40021000	4.60906200
H	-4.54476700	-1.85958600	1.86861800
H	-2.54318500	-4.54857800	-0.08071700
H	-4.49488300	-1.81620000	-2.02064800
H	-5.19906800	1.68401200	1.70836600
H	0.68295000	5.08202800	0.06598000
H	-2.53247200	4.11195600	1.93933500
H	-2.48193300	4.15437800	-1.90909000
H	-0.42412200	3.09478700	4.69411300
H	-0.38400500	-4.78255400	-2.95864000
H	-0.30293000	3.19724100	-4.62884900
H	3.92870500	0.68667400	-3.10070800
O	5.72377900	0.02054600	-0.05670600
H	6.20869500	-0.42808600	0.65226100

$Si_{29}H_{24}$-H_2O

Si	-0.14142300	-2.86185700	2.97679800
Si	2.28479900	0.69017400	3.18538300
Si	1.87348000	-1.61527900	2.76196500
Si	-1.99053200	0.97987000	3.62355600
Si	-1.97164100	-1.35199500	3.15184800
Si	1.68964400	-1.35565800	0.46507500
Si	3.37886400	1.56659800	1.09922600
Si	1.40918400	-3.41400200	-0.56356900
Si	3.57518400	-0.30909700	-0.36661200
Si	-0.44746100	-4.04882600	0.78109000
Si	-2.21937800	-1.08429400	0.86314300
Si	-0.00520400	2.16576700	1.05730600
Si	0.20947500	1.84163300	3.34214000
Si	-2.43488000	-3.14867600	-0.16715400
Si	-0.24884400	0.01099300	-0.00559200
Si	-3.37585000	2.03273300	1.80787700
Si	-4.06478400	0.24059700	0.40378300
Si	2.87927600	-0.45707900	-2.64705900
Si	1.46171800	-2.53082900	-2.77396900
Si	-0.48403000	0.29982100	-2.39354000
Si	1.02284400	3.38112400	-2.00852000
Si	1.88922800	3.18788400	0.19880200
Si	-0.72163000	-1.79179100	-3.36390600
Si	1.42406900	1.35025800	-3.18198700
Si	-2.81806200	-2.24473400	-2.33366600
Si	-3.89890800	-0.00567300	-1.95663800
Si	-1.47201500	3.54712900	-1.74824700
Si	-1.88757800	3.43521600	0.59168900
Si	-2.35836200	1.60241300	-2.79285000
H	-0.53147700	-5.52385600	1.01986700
H	-3.71693800	-3.09388700	-3.17649200
H	3.06968800	-2.45162400	3.08141100
H	3.17977700	0.92760900	4.36125600
H	4.71306500	2.16646000	1.46315100
H	2.59849400	-4.27611100	-0.28885100
H	4.01639600	-0.57518800	-3.61527500
H	-1.74999200	4.77867400	1.23554100
H	0.36960600	3.16768600	4.01630800
H	2.07213800	4.52692800	0.84124800
H	1.53041400	4.59036600	-2.73046700
H	-2.58270100	1.31038600	4.95753500
H	-4.52030800	2.77868100	2.41865600
H	-5.29359100	-0.42607100	0.93662700
H	-3.18917500	-2.02627900	3.70114500
H	-3.65510200	-3.83458500	0.36126300
H	-5.22571200	0.03399500	-2.64769300
H	1.30940300	1.55192300	-4.66045700
H	-2.51831800	1.80145500	-4.26696400
H	-0.86692600	-1.63139900	-4.84438000
H	-1.95215600	4.82058000	-2.37074100
H	-0.10319700	-3.86405500	4.08759900
H	2.04387200	-3.48259500	-3.77102900
O	4.94121600	-1.21504800	-0.03991400
H	5.77456200	-0.69151200	-0.03785900
O	7.01342400	0.64350300	0.04039600
H	7.15056200	1.10691100	-0.80034800
H	6.63994700	1.31397800	0.63590000

Section 15. The $Si_{29}H_{24}$ cluster with two terminal hydroxyl groups.

The $Si_{29}H_{24}$ cluster, a "reconstructed" tetrahedral model, was chosen to conduct the research. Here we performed the two different substitution sites for the $Si_{29}H_{24}$ cluster terminated with two hydrophilic hydroxyl groups. One case is when the two terminal hydroxyl groups are relatively close, and the other is when two terminal hydroxyl groups are far away from each other. The modified structures, the photoluminescence, and absorption spectra of these structures are presented in the following part. As shown in Figure 5, the absorption wavelength of $S_0 \rightarrow S_1$ for both substitution cases is around 400nm and is not related to the distances between the two hydroxyl groups. Similarly, the photoluminescence spectra reveal a single peak around 550 nm for both cases (Figure S15b). Thus, the excitation and emission properties of the $Si_{29}H_{24}$ cluster modified by two hydroxyl groups do not differ at different positions. However, the situation may be different when more hydrogen atoms are replaced, which can be investigated in the future.

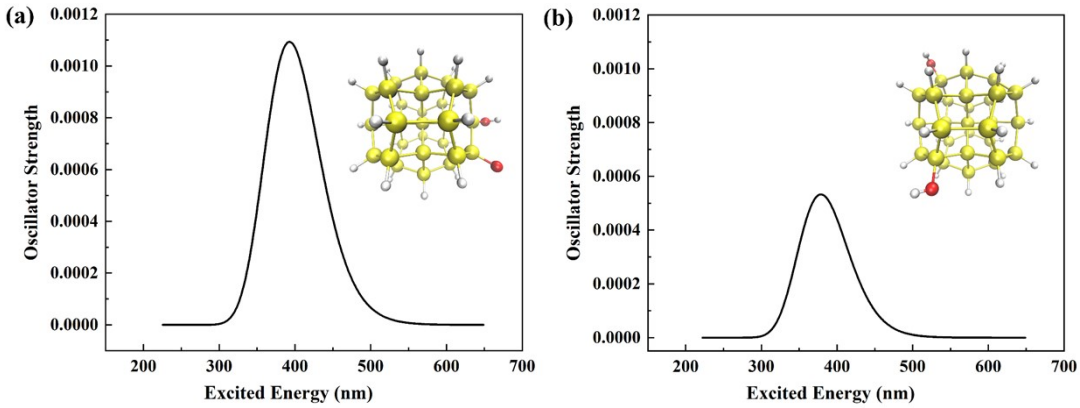

Figure S15a. The absorption spectra of $Si_{29}H_{24}$ with two close terminating hydrophilic hydroxyl (a) and two distant terminating hydrophilic hydroxyl groups (b)) and the corresponding structures are inserted in the plots.

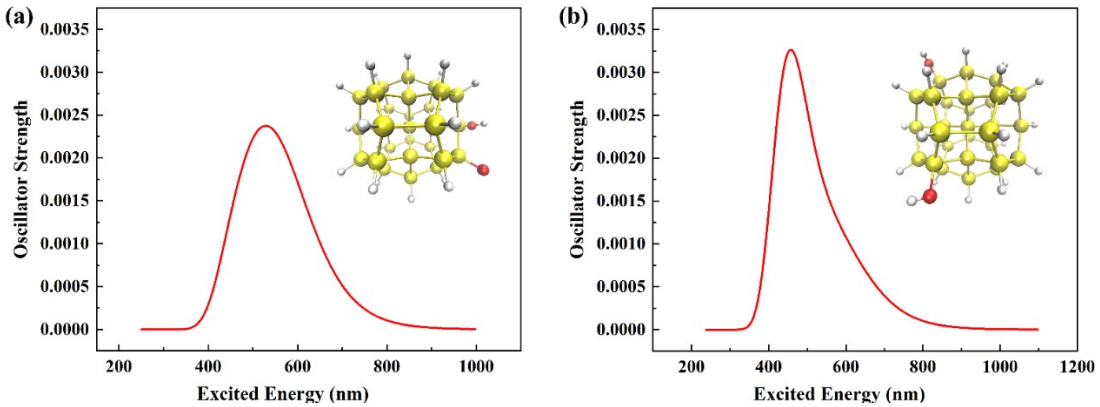

Figure S15b. The photoluminescence spectra of $Si_{29}H_{24}$ with two close terminating hydrophilic hydroxyl (a) and two distant terminating hydrophilic hydroxyl groups (b) and the corresponding structures are inserted in the plots.

The cartesian coordinates of $Si_{29}H_{24}$ with two close terminating hydrophilic hydroxyl as shown below:

Si -3.76400600 -1.24559000 0.02937900

Si	-2.42545800	1.99363300	-2.48881500
Si	-3.45933600	1.05409300	-0.55688700
Si	-1.18025600	-2.06201300	-3.31319600
Si	-2.33686100	-2.59806300	-1.30645700
Si	-1.61676100	1.36732100	0.80542300
Si	-0.76615600	3.67274300	-1.63618900
Si	-2.10836500	0.74468100	2.98529700
Si	-0.94934500	3.58787400	0.73424600
Si	-2.86203000	-1.42994700	2.38797800
Si	-0.48083400	-2.32116100	0.05813500
Si	0.73388700	0.62382000	-2.27128900
Si	-1.14946000	0.30428400	-3.58166700
Si	-0.98587500	-2.88532400	2.24982800
Si	0.19482500	-0.00652600	-0.00388100
Si	1.20969100	-2.73507200	-2.92986600
Si	1.27987700	-3.61288000	-0.71983500
Si	0.74948400	3.32510900	2.37893200
Si	-0.01543400	1.44887200	3.86731400
Si	2.13001900	0.31150000	1.40715200
Si	3.32811300	2.50337300	-0.97861600
Si	1.37065300	2.85257400	-2.28416400
Si	1.57261500	-0.29845500	3.57244100
Si	2.73650600	2.54694500	1.32554600
Si	1.23517400	-2.59462900	3.04907300
Si	2.73218600	-3.07479500	1.08626300
Si	4.05675000	0.14417700	-1.45641400
Si	2.47269400	-0.72008600	-3.00675600
Si	3.84247100	-1.02724200	0.60312300
H	-3.94155200	-1.94176500	3.29323600
H	1.58562500	-3.51195800	4.17832500
H	-3.39752500	2.67015800	-3.40755300
H	-1.07456400	5.02404200	-2.20075400
H	-2.05510900	4.46292300	1.23006000
H	-3.22926500	1.58964900	3.50065600
H	0.96617700	4.55587300	3.20208200
H	2.82427000	-0.34918900	-4.41279000
H	-0.84245400	0.68453800	-4.99576000
H	1.71071900	3.25925500	-3.68324700
H	4.43850400	3.44688500	-1.31943000
H	-1.71460300	-2.77758100	-4.51379300
H	1.62222500	-3.72734500	-3.97131400
H	0.88457900	-5.05536000	-0.69198700
H	-2.75418000	-4.03364900	-1.26129000
H	-1.40292900	-4.32114000	2.30275000
H	3.67224000	-4.18532500	1.43583800
H	3.93699300	2.76401900	2.19175500
H	5.05401000	-0.84733300	1.46223100
H	2.76367300	-0.11063300	4.45818000
H	5.45636100	0.15179200	-1.98598600
H	-0.09292700	1.93350700	5.28119600
O	-5.34697300	-1.82649900	-0.05855200
H	-5.96015300	-1.46099500	0.59702900
O	-4.72949300	2.01109600	0.03464400
H	-5.46517000	2.13382900	-0.58353500

The cartesian coordinates of $Si_{29}H_{24}$ with two distant terminating hydrophilic hydroxyl groups as shown below:

Si	1.91824700	3.54656200	0.05865100
Si	-1.75124800	2.97952100	-2.13038900
Si	0.60842500	3.18405400	-1.89351000
Si	-1.78962800	2.93185600	2.17095400
Si	0.57282700	3.14076300	1.97557700
Si	1.00349200	0.90073400	-1.95214700
Si	-2.12706200	0.85261400	-3.41769000
Si	3.28001300	0.45393700	-1.90970100
Si	0.03729300	-0.04218000	-3.83699600
Si	3.69849200	1.74587800	0.03959900

Si	0.96897700	0.85661600	1.98257600
Si	-2.39644500	0.32454500	-0.01522300
Si	-2.74163700	2.60697300	0.00754700
Si	3.24555500	0.40994900	1.96674500
Si	-0.01714500	-0.09093300	-0.00351400
Si	-2.18297200	0.77791800	3.40414800
Si	-0.02430500	-0.12476100	3.83424500
Si	0.88504600	-2.22692500	-3.42723900
Si	3.02619000	-1.89806700	-2.15193600
Si	0.36468800	-2.47492200	-0.02217200
Si	-2.81931900	-2.84397100	-1.31074800
Si	-3.29916600	-0.59984900	-1.94010300
Si	2.65025700	-2.85651900	-0.00559700
Si	-0.58505700	-3.36233500	-1.94123100
Si	2.98877800	-1.94600700	2.16808100
Si	0.82740500	-2.30203500	3.39783100
Si	-2.84018900	-2.87104000	1.20535500
Si	-3.32940300	-0.64088000	1.87495300
Si	-0.61684800	-3.40268100	1.86168200
H	4.10719000	-2.60244600	2.91468200
H	1.22666000	3.82943900	-3.09350900
H	-2.36641400	4.12723100	-2.87154500
H	-2.88668900	1.15261700	-4.67150500
H	0.65054000	0.55973700	-5.06160200
H	3.91153500	1.08018400	-3.11208000
H	1.16284700	-2.99264700	-4.68259400
H	-4.80235300	-0.38793100	1.89158300
H	-4.77188400	-0.34771200	-1.97611900
H	-3.81914800	-3.82945900	-1.82886100
H	-2.41709100	4.06341300	2.92654000
H	-2.96151600	1.04895100	4.65293400
H	0.57262600	0.45492500	5.07771600
H	1.17390400	3.75053500	3.20362600
H	3.84859400	1.01269500	3.19954000
H	1.08087900	-3.09344500	4.64245600
H	-0.34971500	-4.83973700	-1.96598300
H	-0.38047600	-4.88015100	1.85717100
H	2.89748300	-4.33198700	-0.02002600
H	-3.84844100	-3.86708800	1.68569500
H	2.58079800	4.89061300	0.08267000
H	4.15627900	-2.53930000	-2.89373200
O	5.24027100	2.42226100	-0.05665000
H	5.48835400	3.01583000	0.66802000
O	-4.40981400	2.89016200	-0.00372700
H	-4.67126000	3.82294500	0.00147600

Section 16. The cartesian coordinates of the optimized structures

The following are the cartesian coordinates of the structures of Si QDs passivated with pure H (Si-H), one F (Si-F), one Si=O (Si-Si=O), and one OH (Si-OH) in the water and vacuum environment. For example, Si-F-1H_2O indicates that the silicon cluster with the F group is in the environment of one water molecule. All the cartesian coordinates of the optimized structures are shown below.

Si-H-vac

Si	3.95661100	-2.36214700	0.32636000
Si	0.99355500	-4.26515600	1.46845600
Si	2.30817400	-2.37596000	2.02683800
Si	1.59094900	-3.76598700	-2.15090300
Si	2.93071600	-1.85531600	-1.74720300
Si	1.04567200	-0.35550000	2.11827200
Si	-2.19176600	-2.26387000	3.37778400
Si	2.48499900	1.48616300	2.58835200
Si	-0.64176200	-0.52237600	3.79458900
Si	4.14731100	1.80867900	0.93236000
Si	1.67410300	0.17017600	-1.69571000
Si	-1.44783500	-1.83544600	-0.49177500
Si	-0.15891200	-3.84017500	-0.55642400
Si	3.10664300	2.00658000	-1.18590400
Si	-0.00019200	0.00014700	0.00007300
Si	-0.91676200	-1.19576900	-4.36658200
Si	0.60911100	0.52444600	-3.79932100
Si	-2.02542600	1.39643400	3.90997200
Si	1.35178500	3.56569900	2.60728800
Si	-1.27201400	2.02125900	0.06934400
Si	-4.39145300	-0.00866400	1.43363900
Si	-3.10903600	-1.98736100	1.21178300
Si	0.19136300	3.83832500	0.56081900
Si	-2.93545200	1.82933100	1.76675300
Si	1.94759900	4.06465000	-1.01199600
Si	-0.74945100	2.46413900	-3.83459800
Si	-3.71211800	0.56125700	-2.69196000
Si	-2.48054300	-1.45989800	-2.60761200
Si	-2.30602100	2.35653300	-2.05272000
H	4.82362400	3.10826500	1.22302400
H	2.90596600	5.07467000	-0.47139700
H	5.09558300	-1.45941500	0.63882200
H	2.96172000	-2.59691600	3.35443000
H	1.92754800	-5.40440800	1.22233900
H	-3.30754200	-2.11533500	4.35954400
H	0.01545600	-0.74498600	5.12010200
H	3.13845000	1.26114800	3.91531700
H	-3.16243200	1.07495900	4.82361100
H	-3.38690700	-2.61041100	-2.91302800
H	-1.06755300	-4.98810900	-0.86475200
H	-4.01427100	-3.13751500	0.90170300
H	-5.22417900	-0.14976200	2.66550400
H	2.44827700	-4.96924100	-1.93180800
H	-1.67147000	-0.74550600	-5.57423600
H	1.65910100	0.63081100	-4.85983500
H	3.97837300	-1.74610800	-2.80973700
H	4.15378200	2.11099300	-2.24945100
H	-1.52613900	2.44446700	-5.11023100
H	-3.73088800	3.09582300	1.80825200
H	-3.10172300	3.62269900	-2.00689500
H	-0.60723600	5.10277400	0.60373700
H	-4.10777400	0.78620700	-4.11453400
H	0.04464900	3.72083700	-3.82765000
H	1.47741700	4.57136300	-2.32801000

H	4.50987200	-3.74589500	0.22651800
H	5.19655800	0.75600500	0.95971500
H	0.46993800	3.72759300	3.79305200
H	-1.32500200	2.57502200	4.48459800
H	-5.32687400	0.19906600	0.29706600
H	-4.96596700	0.50287900	-1.89552900
H	-0.23840700	-2.46857100	-4.72650200
H	1.09504400	-3.83390000	-3.55067900
H	0.08450500	-4.67731000	2.57006900
H	-1.60639700	-3.61456600	3.58504800
H	2.38704000	4.63969100	2.68214100

Si-H-1H_2O

Si	-3.97414800	1.78531900	-0.98562100
Si	-2.55256900	-0.27163000	-3.70755200
Si	-2.18312000	1.75371500	-2.53573200
Si	-4.01188500	-1.89999900	-0.72810200
Si	-3.69575200	0.04026400	0.59184700
Si	-0.03920700	1.84764300	-1.49830100
Si	1.61457000	-0.32082200	-4.37600900
Si	0.18050200	3.87663800	-0.26654300
Si	1.67507100	1.70386600	-3.14867900
Si	-1.42790400	4.07777600	1.45975600
Si	-1.55569600	0.12082800	1.64463100
Si	-0.04852000	-2.04563500	-1.21552100
Si	-2.19798500	-2.09933200	-2.24274300
Si	-1.31955400	2.16408600	2.85066200
Si	0.16847800	-0.00114000	-0.00094600
Si	-1.44763100	-3.81820200	2.02889700
Si	-1.32802900	-1.72696200	3.13407700
Si	3.85061200	1.68711300	-2.21232600
Si	2.23494600	4.03459700	0.90085200
Si	2.30587000	0.07362900	1.06179200
Si	3.84211600	-2.00559000	-1.94415600
Si	1.66602400	-2.14668400	-2.86867700
Si	2.49795000	2.12011300	2.26971700
Si	3.99894900	-0.05287000	-0.61241000
Si	0.79479000	2.39709600	3.89226800
Si	0.78491800	-1.80952100	4.20043200
Si	2.22077600	-3.86646600	1.48166800
Si	0.16892500	-3.87298700	0.29938600
Si	2.49021100	-1.77397500	2.55712800
H	-1.05471600	5.26244000	2.28936000
H	0.88941100	3.79589500	4.40767700
H	-4.18123700	3.11658500	-0.35502300
H	-2.32337400	2.91210400	-3.47228500
H	-3.98881400	-0.29234200	-4.11841300
H	2.85995200	-0.38237100	-5.19836800
H	1.54312500	2.86238500	-4.08624800
H	0.04948000	5.03048900	-1.21004500
H	4.80923100	1.36797500	-3.31239200
H	0.03844300	-5.15098100	-0.46755100
H	-2.32859500	-3.37525900	-3.01363500
H	1.52998500	-3.42671200	-3.63119200
H	4.80406800	-1.85399600	-3.07668600
H	-5.22795000	-1.70189900	-1.56592600
H	-1.08642800	-4.87498800	3.02060700
H	-2.40508900	-1.64716000	4.16960200
H	-4.72258900	0.14270800	1.66963000
H	-2.39650600	2.24335800	3.88667500
H	0.87820100	-3.11878600	4.91328300
H	5.33962700	-0.00698700	0.05023700
H	3.82808400	-1.72235100	3.22492600
H	3.83610200	2.16419000	2.93750700
H	2.12810800	-4.90882400	2.54746500
H	0.95259000	-0.74432200	5.22383700
H	0.96228400	1.49138200	5.05904500

H	-5.21879000	1.50453800	-1.77010200
H	-2.79678200	4.32960200	0.93626400
H	3.39269800	4.25733900	-0.00470600
H	4.24651300	3.00938600	-1.66027100
H	4.23049500	-3.23539900	-1.20462800
H	3.37983600	-4.22444200	0.62241400
H	-2.81627800	-4.12779400	1.53823900
H	-4.21828300	-3.12462800	0.08756000
H	-1.74426000	-0.35933800	-4.95214100
H	0.46691700	-0.38572600	-5.31869900
H	2.14892100	5.22308100	1.80144900
O	-7.18886800	-0.08176400	-0.02104900
H	-7.29959900	0.62994800	0.62754100
H	-6.97174500	0.38287700	-0.84377600

Si-H-2H_2O

Si	-3.44994700	-0.65350900	-2.63352500
Si	-0.53773300	-2.70582300	-3.64848200
Si	-1.26835400	-0.45660600	-3.53269800
Si	-2.52156000	-3.65677700	-0.66325000
Si	-3.30518600	-1.43464500	-0.40252200
Si	0.15161400	0.92045500	-2.20196900
Si	3.36526000	-1.15728000	-3.22756300
Si	-0.74406300	3.12435300	-2.06676800
Si	2.34220500	0.97710200	-3.14045100
Si	-2.88777000	3.21838100	-1.06015400
Si	-1.91162800	-0.05610300	0.95329900
Si	1.15704800	-2.21322500	-0.10780500
Si	-0.28630900	-3.55233300	-1.45129400
Si	-2.81123100	2.15065500	1.05079500
Si	0.27503300	0.00301900	-0.00044000
Si	-0.83995900	-3.15092100	3.17704600
Si	-1.77118600	-0.97375300	3.14927000
Si	3.86872300	2.24111500	-1.84384100
Si	0.53820600	4.55679700	-0.68375000
Si	1.69020900	1.36787600	1.35519500
Si	4.82385200	-0.73012100	0.14615200
Si	3.33848000	-2.12232000	-1.06483100
Si	0.77111800	3.56570600	1.45386500
Si	3.86485200	1.42315600	0.37905500
Si	-1.43900000	3.61814100	2.30618000
Si	-0.32246700	0.24212400	4.57466900
Si	2.59265200	-1.80155600	3.56439500
Si	1.26813100	-3.10759000	2.09907800
Si	1.80164400	0.43079400	3.54493200
H	-3.17300200	4.66908000	-0.84145400
H	-1.95709900	5.00518400	2.10559700
H	-4.23269400	0.60657500	-2.74477400
H	-1.35271100	0.12216300	-4.91003500
H	-1.61980600	-3.49086400	-4.31536700
H	4.79450200	-0.95295700	-3.61054200
H	2.26280700	1.55145200	-4.51983300
H	-0.81521800	3.70050800	-3.44643200
H	5.23338900	2.00747700	-2.40439100
H	1.82223100	-4.49560300	2.02937800
H	0.28191500	-4.93497600	-1.52343600
H	3.89772800	-3.50841600	-1.13090100
H	6.06598200	-0.58100200	-0.66995200
H	-3.31028300	-4.29320100	-1.75715400
H	-0.60920000	-3.52389700	4.60475700
H	-3.14355400	-1.00927200	3.74455200
H	-4.67889700	-1.42776400	0.19881700
H	-4.17178100	2.08247300	1.65515600
H	-0.14628700	-0.55903700	5.82290000
H	4.75462800	2.27699600	1.22635200
H	2.69299900	1.28557300	4.38962500
H	1.65421700	4.42043200	2.30740800
H	2.39461800	-2.33374700	4.94591400

H	-0.88344700	1.55840900	4.97767500
H	-1.49223500	3.34336300	3.76622300
H	-4.18259000	-1.68407100	-3.43110200
H	-3.94948800	2.69711100	-1.96188400
H	1.84423600	4.92681900	-1.28976200
H	3.61219000	3.70348500	-1.91993600
H	5.22797800	-1.31953300	1.44968900
H	4.04554900	-1.89902200	3.26485200
H	-1.75537400	-4.16973400	2.60016100
H	-2.64932400	-4.48089800	0.56158200
H	0.68568800	-2.86152000	-4.47849700
H	2.76068200	-2.04039400	-4.25938400
H	-0.23580300	5.82302500	-0.51080800
O	-5.79992300	-4.23345800	0.04661400
H	-5.97721900	-4.04965700	-0.88837200
H	-5.86435100	-3.36377700	0.47002300
O	-6.01124000	3.95372400	0.08081600
H	-6.23446400	3.65708100	-0.81462900
H	-5.64407100	4.84042700	-0.05572200

Si-H-3H_2O

Si	-3.47357100	-2.39540700	-0.64203100
Si	-0.66278700	-4.42486300	0.70275400
Si	-1.32777100	-3.22092300	-1.22451800
Si	-2.46992900	-2.06724800	2.90670500
Si	-3.20845600	-0.77351000	1.06441600
Si	0.21490800	-1.50792900	-1.83259700
Si	3.29268400	-3.61043300	-0.49450700
Si	-0.60676900	-0.29707400	-3.71594400
Si	2.34578100	-2.45426000	-2.33178500
Si	-2.66997800	0.79288000	-3.29979600
Si	-1.67626600	0.96929900	0.50682000
Si	1.26326700	-1.18960800	1.90961200
Si	-0.29647400	-2.90048600	2.47619400
Si	-2.44696800	2.18177000	-1.39738400
Si	0.45088500	0.00043800	0.00338800
Si	-0.52833300	1.41280900	4.28980800
Si	-1.41581800	2.45221500	2.35542900
Si	4.00457800	-0.83789200	-2.82956200
Si	0.82780100	1.47388700	-4.35780500
Si	2.00733800	1.71980400	-0.57263000
Si	4.98864800	-0.55690700	0.73143700
Si	3.37409200	-2.16302100	1.37902100
Si	1.20524200	2.88222800	-2.49171700
Si	4.12063600	0.72881100	-1.05752900
Si	-0.92614100	3.84303600	-2.13472300
Si	0.14678900	4.17999200	1.92876500
Si	2.94557200	2.14808000	3.24674900
Si	1.50263000	0.33236600	3.72867100
Si	2.20998000	3.22132300	1.26817300
H	-2.95156900	1.67145100	-4.47622300
H	-1.41947400	4.34073300	-3.45469300
H	-4.19926000	-1.90071000	-1.83709900
H	-1.45457000	-4.17076200	-2.37482200
H	-1.80348400	-5.30490400	1.09811700
H	4.70173100	-3.95051100	-0.85577200
H	2.20107700	-3.39185300	-3.48893300
H	-0.76924100	-1.24404800	-4.86344600
H	5.31737600	-1.54809600	-2.88968600
H	2.01795500	-0.41245600	4.91970800
H	0.20760000	-3.63396300	3.67910700
H	3.86973900	-2.91779800	2.57220300
H	6.18099900	-1.29533400	0.21741000
H	-3.38280900	-3.24365000	3.02769200
H	-0.20868700	2.49326900	5.27067900
H	-2.74574800	3.05641400	2.68364300
H	-4.52203700	-0.15325700	1.41752700
H	-3.74539100	2.84135800	-1.07372900

H	0.38196900	4.90341300	3.21443900
H	5.09017300	1.81217500	-1.41154700
H	3.17063200	4.30931100	0.90431400
H	2.18921600	3.94830300	-2.85805700
H	2.81997100	3.12939200	4.36595800
H	-0.36036800	5.18106000	0.95373900
H	-0.87588700	5.01838700	-1.22494400
H	-4.22948400	-3.54702800	-0.07232200
H	-3.79889100	-0.16731400	-3.19958900
H	2.08716400	0.99124300	-4.98340300
H	3.80115600	-0.18939000	-4.15181700
H	5.45299000	0.28051300	1.86874900
H	4.37484500	1.74423300	3.18135800
H	-1.49942300	0.50129400	4.95068800
H	-2.55284300	-1.32504400	4.19303200
H	0.50538500	-5.31262600	0.46276700
H	2.59862000	-4.89181000	-0.20103700
H	0.11277700	2.28477400	-5.38885800
O	-6.75761200	-1.52398600	-0.23336900
H	-7.53992100	-2.03143500	-0.49516800
H	-7.05643800	-0.92672900	0.49721800
O	-6.00276500	0.92932300	-1.15969500
H	-6.20936100	-0.03595700	-1.13682000
H	-6.39869600	1.26664400	-1.97685000
O	-7.30220200	0.68818300	1.25643000
H	-6.89215300	1.09318000	0.45658400
H	-6.64698400	0.82806000	1.95709300

Si-H-4H_2O

Si	-2.39093600	0.40458800	-3.42530300
Si	-3.60890400	-1.70781600	-0.64044400
Si	-1.95428900	-1.65416100	-2.33968100
Si	-3.54565100	1.95200400	-0.27780300
Si	-1.88039400	2.18698900	-1.95142600
Si	0.28259300	-1.80054900	-1.53064400
Si	-0.85021700	-4.09714100	1.47891700
Si	1.83236900	-1.62740500	-3.33342600
Si	0.59543000	-3.86505400	-0.38161800
Si	1.68900900	0.43257900	-4.49253400
Si	0.35682600	2.08168600	-1.13898800
Si	-0.89663400	-0.15264400	1.78830100
Si	-3.12723700	-0.02618900	0.95572200
Si	1.90583600	2.21293000	-2.94583000
Si	0.66347100	0.00038700	-0.00912100
Si	-0.71004900	3.76887800	2.26622900
Si	0.74097800	3.86309700	0.39792800
Si	2.74633300	-4.08172500	0.58495900
Si	4.08687300	-1.66418800	-2.60858600
Si	2.89067200	-0.12671300	0.84158300
Si	1.62475400	-2.51602300	3.73783000
Si	-0.57549700	-2.23132200	2.91045800
Si	4.41575900	0.02811700	-0.98420500
Si	3.16984300	-2.20774300	1.96999300
Si	4.15753400	2.02160700	-2.23643700
Si	2.89526400	3.80251700	1.37900500
Si	1.69964500	1.68113900	4.16111100
Si	-0.50618500	1.64835600	3.29966300
Si	3.24013700	1.67612400	2.36233400
H	2.85581300	0.50324700	-5.42307300
H	5.00739100	1.89812400	-3.45864200
H	-1.70435900	0.51888100	-4.73923400
H	-2.18659700	-2.77621700	-3.30273900
H	-4.88904100	-1.34411000	-1.31914600
H	-0.42810100	-5.31568000	2.23348900
H	0.35924100	-4.99150800	-1.33764100
H	1.59640800	-2.75392700	-4.28947100
H	2.72044100	-5.28846100	1.46507900
H	-1.48292000	1.55115000	4.42904000

H	-4.04216800	-0.12542100	2.12638900
H	-1.54630900	-2.32869700	4.04528300
H	1.75049700	-3.93127600	4.19886900
H	-4.82383800	1.77022400	-1.02734000
H	-0.26013900	4.80113400	3.24762600
H	0.55356600	5.16476500	-0.31577200
H	-2.06809400	3.48783100	-2.66785700
H	1.71611300	3.51680300	-3.65485800
H	2.91808000	4.81345200	2.47850500
H	4.56501600	-2.28626600	2.50471400
H	4.63438400	1.59341100	2.89904900
H	5.81389400	-0.05259200	-0.45743200
H	1.87727500	2.96850900	4.89785100
H	3.97101200	4.17562800	0.42301200
H	4.62868400	3.22380000	-1.49950600
H	-3.85926000	0.46077200	-3.70309700
H	0.46226000	0.54015000	-5.32512300
H	4.51225100	-3.00603600	-2.12988200
H	3.81212900	-4.30214500	-0.42793700
H	1.91273000	-1.64903500	4.91079200
H	1.95037800	0.58583800	5.13467900
H	-2.11603700	4.09282000	1.90675900
H	-3.68992300	3.16770900	0.56326200
H	-3.78297400	-3.06306900	-0.05834200
H	-2.26671700	-4.30171300	1.07575300
H	4.94367300	-1.32876200	-3.78531200
O	-7.76627500	1.42148800	-1.08488700
H	-7.85489500	0.44375600	-1.25231000
H	-7.09597600	1.72394100	-1.71619600
O	-6.62782300	1.28418500	1.33795300
H	-7.13869100	1.80745400	1.97298900
H	-7.06331600	1.44054800	0.45158900
O	-7.84044500	-1.29133600	-1.22931200
H	-7.16359700	-1.67059000	-1.80998700
H	-7.49513000	-1.46673000	-0.31666100
O	-6.66010600	-1.41708100	1.21654400
H	-7.06377300	-1.83671700	1.99007300
H	-6.64488400	-0.44158300	1.40856200

Si-H-5H_2O

Si	2.58103200	-2.93290000	-1.09052600
Si	3.68522100	0.61175500	-0.95034200
Si	2.28526300	-0.85146600	-2.18144100
Si	3.06869500	-1.27967500	2.17148500
Si	1.63043900	-2.80980200	1.07660500
Si	0.00308700	-0.16383300	-2.24432200
Si	1.02105600	3.66151900	-2.13142100
Si	-1.31711800	-1.75454100	-3.43237400
Si	-0.17586700	1.97395800	-3.28410800
Si	-1.31129600	-3.90246600	-2.43405500
Si	-0.65455500	-2.13558100	1.05276700
Si	0.51033100	1.57733500	1.20091300
Si	2.79094500	0.87383300	1.22329300
Si	-1.96854000	-3.70598000	-0.16725000
Si	-0.81430600	-0.00101300	-0.00576700
Si	-0.29030700	-0.35411800	4.56635500
Si	-1.47276000	-1.95562700	3.28416500
Si	-2.38647700	2.82273300	-3.30413200
Si	-3.62140400	-1.20623000	-3.46587000
Si	-3.09527200	0.70669100	-0.03284400
Si	-1.90394900	4.48396700	-0.02874700
Si	0.32577200	3.70085200	0.13195700
Si	-4.38301600	-0.89256600	-1.24484200
Si	-3.23312100	2.83761200	-1.09268800
Si	-4.24502300	-3.07375100	-0.33218600
Si	-3.70713600	-1.17968400	3.40057800
Si	-2.60331900	2.34746100	3.54004100
Si	-0.32139700	1.72380100	3.43033300

Si	-3.88315800	0.86124500	2.21225700
H	-2.34692900	-4.72324100	-3.13104700
H	-4.90505600	-4.00584100	-1.29508200
H	2.03897300	-4.06922900	-1.88243700
H	2.78318500	-0.95435500	-3.58992400
H	5.00026500	-0.06516300	-0.82194300
H	0.64157000	4.97372900	-2.73577400
H	0.32925400	1.87384900	-4.68950000
H	-0.81026700	-1.85560400	-4.83705500
H	-2.32035400	4.24067000	-3.76940100
H	0.49936900	2.71744200	4.19170600
H	3.56265300	1.89110600	1.99744100
H	1.14611300	4.69983500	0.88585500
H	-1.89674700	5.69268800	-0.90712000
H	4.45686800	-1.74500100	1.90307800
H	-1.02268500	-0.17494600	5.85624500
H	-1.37632300	-3.29500600	3.94375200
H	1.72206000	-4.14788700	1.74202100
H	-1.87116900	-5.04272100	0.49840700
H	-4.00938400	-0.88981500	4.83466500
H	-4.66232500	3.28076500	-1.10759400
H	-5.31096400	1.30911100	2.19613200
H	-5.81217400	-0.44934600	-1.26560300
H	-3.04976200	2.18044200	4.95585100
H	-4.69318500	-2.19578700	2.94700700
H	-4.97010800	-3.20069400	0.95973600
H	4.04659700	-3.15913400	-0.93382200
H	-0.01436500	-4.61032100	-2.59726700
H	-3.92349900	-0.04555100	-4.34451700
H	-3.27278100	2.09728400	-4.25218200
H	-2.46125800	4.90694000	1.28300900
H	-2.82592600	3.77329300	3.18152900
H	1.08575600	-0.79945300	4.91012300
H	2.88376500	-1.27312900	3.64838000
H	3.90448700	1.90223300	-1.65567700
H	2.49352400	3.52544700	-2.28255600
H	-4.35545600	-2.37973100	-4.02819500
O	7.47460500	-1.77533900	1.38946800
H	7.26565400	-1.89127100	0.42149600
H	8.43973000	-1.69513700	1.41724100
O	6.35028400	0.59285000	1.97252600
H	6.30099900	0.69290900	2.93323000
H	6.75074100	-0.30608100	1.80354800
O	6.99687500	-1.83763100	-1.26547300
H	7.23992100	-0.91820900	-1.56343300
H	7.54679200	-2.43237900	-1.79610100
O	7.14333900	2.33418900	0.07785300
H	7.90555400	2.83749200	0.39905600
H	6.85446400	1.77161200	0.84312700
O	7.68411300	0.67255300	-1.98816700
H	7.09873800	1.00677400	-2.68420300
H	7.52648000	1.28905300	-1.22153300

Si-F-vac

Si	0.08566700	3.96985700	-2.37487800
Si	2.44180500	3.95690200	0.48671100
Si	0.12719200	3.88775000	-0.00858900
Si	3.26254600	2.10717600	-2.62234900
Si	0.98032200	1.95378200	-3.23763800
Si	-0.94283300	1.95124400	0.87923600
Si	1.47758800	1.84137200	4.01730200
Si	-3.24120200	1.94283200	0.25442200
Si	-0.76215500	1.92893200	3.25456300
Si	-3.56988500	1.86836900	-2.09083100
Si	-0.08884200	0.00064500	-2.38302000
Si	2.41679700	0.00020200	0.62433900
Si	3.45431300	1.95323900	-0.26612500
Si	-2.40322800	-0.00011600	-2.96357900

Si	0.11232300	-0.00000500	-0.00276800
Si	3.26421400	-2.10455300	-2.62236900
Si	0.98222300	-1.95098600	-3.23872200
Si	-1.76451400	-0.00203900	4.18625600
Si	-4.41052800	-0.00050200	0.93499700
Si	-0.94221100	-1.95215500	0.87798600
Si	1.47893800	-1.84220500	4.01639900
Si	2.57091700	0.00023800	3.00510300
Si	-3.24083800	-1.94352700	0.25421200
Si	-0.76060400	-1.93156300	3.25325000
Si	-3.56922100	-1.86911900	-2.09106500
Si	0.08780200	-3.96806000	-2.37805500
Si	2.44221600	-3.95692500	0.48488400
Si	3.45484600	-1.95259600	-0.26598500
Si	0.12791300	-3.88775600	-0.01166100
H	-5.02352300	1.66542500	-2.35148700
H	-5.02286600	-1.66691700	-2.35221300
H	-1.26286400	4.28565100	-2.91439200
H	-0.54372600	5.10332000	0.54877600
H	3.03630900	5.08495600	-0.29093200
H	1.44206400	1.58580800	5.48857200
H	-1.43264400	3.14979000	3.80100000
H	-3.90296100	3.15641100	0.82738600
H	-1.51588100	-0.00235900	5.65842700
H	4.90050300	-1.94893600	0.11950200
H	4.90015400	1.94960400	0.11867100
H	4.01529700	0.00067500	3.39548900
H	1.44255800	-1.58720500	5.48775100
H	3.74287700	3.46424100	-3.02108900
H	3.74470800	-3.46123200	-3.02223400
H	0.86923500	-1.95064300	-4.73069100
H	0.86648300	1.95468600	-4.72954500
H	-2.51679700	-0.00001200	-4.45561300
H	0.99973500	-5.07314700	-2.80040800
H	-1.42999700	-3.15327500	3.79912600
H	-0.54307600	-5.10385200	0.54446300
H	-3.90237400	-3.15725500	0.82710800
H	3.03742700	-5.08429200	-0.29321600
H	-1.26020400	-4.28404400	-2.91879000
H	-3.17401500	-3.13762900	-2.75792700
H	0.99678600	5.07562700	-2.79720200
H	-3.17566000	3.13702700	-2.75798000
H	-4.80026400	-0.00058400	2.37069800
H	-3.24004100	-0.00247900	3.99100800
H	2.19881700	-3.12699500	3.81368800
H	2.71023000	-4.22851000	1.92180100
H	4.11994100	-1.11487200	-3.32827500
H	4.11789500	1.11817600	-3.32966400
H	2.71077800	4.22745500	1.92364500
H	2.19599200	3.12697100	3.81462200
F	-5.81141700	-0.00084900	0.08795600

Si-F-1H_2O

Si	-1.18246300	-3.42920300	-2.95869600
Si	-3.49100000	-3.29377900	-0.06067000
Si	-1.22479900	-3.71228100	-0.60780700
Si	-3.81754400	-0.83829900	-2.81549900
Si	-1.56268000	-1.14870700	-3.47215900
Si	0.27120000	-2.25434800	0.54051400
Si	-2.08111600	-2.05078500	3.72462900
Si	2.51251700	-2.69194200	-0.13820300
Si	0.07641500	-2.56251400	2.89486000
Si	2.86572500	-2.32780000	-2.45312600
Si	-0.06413100	0.33314700	-2.35759900
Si	-2.50476800	0.47016900	0.68891600
Si	-3.97927700	-1.01081000	-0.45854700
Si	2.18677100	-0.12429200	-2.99711400
Si	-0.26605700	0.00669300	-0.00155500

Si	-2.79627500	3.20252200	-2.16506400
Si	-0.61933600	2.59377900	-2.87297000
Si	1.50710200	-1.10372500	4.08955200
Si	4.10634400	-1.22545400	0.82124100
Si	1.24055400	1.47197500	1.12621900
Si	-1.16508800	1.47913500	4.28466200
Si	-2.67305400	0.13874900	3.04431200
Si	3.48901000	1.03149700	0.45866400
Si	1.03285300	1.13265700	3.47576600
Si	3.78111200	1.23046900	-1.88431300
Si	0.75233200	4.16156200	-1.74686000
Si	-1.54797500	4.28460700	1.15262600
Si	-3.02500300	2.73190000	0.14471000
Si	0.68075500	3.72427500	0.57939800
H	4.32783500	-2.43835100	-2.72588900
H	5.12541600	0.69596900	-2.25210400
H	0.05797900	-3.96313700	-3.57959900
H	-0.87724800	-5.12611300	-0.26412600
H	-4.33430300	-4.10352800	-0.98991100
H	-1.99908300	-2.04986500	5.21594100
H	0.42056000	-3.98077700	3.22370500
H	2.86640600	-4.10198600	0.21476200
H	1.22775500	-1.26272300	5.54743800
H	-4.42745700	3.02118400	0.57792300
H	-5.38382200	-0.72070100	-0.03271000
H	-4.07544000	0.43342400	3.47388900
H	-1.20419800	1.00058700	5.69903300
H	-4.61232500	-1.95902400	-3.40115400
H	-2.92409500	4.68072200	-2.33590500
H	-0.50032400	2.79348400	-4.35086500
H	-1.43996700	-0.94143400	-4.94867800
H	2.31896200	0.08011500	-4.47345800
H	0.15952600	5.51451200	-1.96737300
H	1.97836400	2.05122300	4.18245800
H	1.62561800	4.64028700	1.29040400
H	4.37689000	1.96478400	1.20516900
H	-1.83953500	5.62695300	0.56649500
H	2.13847600	4.20031400	-2.28194000
H	3.74606300	2.64499100	-2.34021400
H	-2.32485800	-4.20943500	-3.52160400
H	2.18513600	-3.35216400	-3.28761300
H	4.46223500	-1.54490800	2.22821600
H	2.94003500	-1.44504500	3.87824900
H	-1.54644800	2.91568500	4.29945600
H	-1.75140400	4.39592100	2.62099500
H	-3.86452500	2.57485900	-2.98638300
H	-4.39754400	0.42685800	-3.33752700
H	-3.83161900	-3.72004200	1.32219800
H	-3.09331500	-3.07064000	3.34365700
F	5.49030300	-1.49465800	-0.04312600
O	7.01776200	0.92618500	0.11240800
H	6.76403000	0.00278600	-0.05084600
H	7.12167700	1.29894300	-0.77565900

Si-F-2H_2O

Si	1.33866300	-4.53601900	-0.19400500
Si	3.33733400	-2.50840100	-2.55973700
Si	1.10884200	-3.18286000	-2.12427900
Si	4.15339900	-2.50781200	1.05927600
Si	1.95482500	-3.17112000	1.64147900
Si	-0.35825900	-1.33017600	-1.81259100
Si	1.67818600	0.94033100	-4.35419300
Si	-2.55801500	-2.07871000	-1.29383300
Si	-0.42034300	0.00505300	-3.78395600
Si	-2.62274900	-3.37407700	0.68778400
Si	0.48896900	-1.32293100	1.99048600
Si	2.62952300	0.79877000	-0.50081700
Si	4.06956000	-1.07313600	-0.82370300

Si	-1.72306400	-2.08482100	2.45779900
Si	0.43737600	-0.00187400	0.00249300
Si	3.43921700	0.94216400	3.37478800
Si	1.29596400	0.02146900	3.78696200
Si	-1.83090700	1.88485600	-3.50675400
Si	-4.12736200	-0.35455000	-0.82349700
Si	-1.03423200	1.84508200	0.33059000
Si	1.04404200	3.94774900	-2.32730600
Si	2.53713100	2.11633400	-2.48656200
Si	-3.24348800	1.09207100	0.82641100
Si	-1.08425600	3.15764400	-1.65672400
Si	-3.28378800	-0.32218300	2.72992500
Si	-0.02719700	1.94787400	4.16971700
Si	1.97581600	3.95814400	1.79132300
Si	3.40067100	2.12539000	1.32343300
Si	-0.22669500	3.16288900	2.14657600
H	-4.04635500	-3.67729400	1.01413600
H	-4.63830600	-0.93867800	2.83512900
H	0.13704900	-5.36819600	0.07542600
H	0.60583300	-4.01221800	-3.26343500
H	4.19466200	-3.73094200	-2.52662300
H	1.44590800	1.93815300	-5.44145400
H	-0.92351700	-0.83008700	-4.91903400
H	-3.06233200	-2.90050700	-2.43995000
H	-1.75063100	2.72902300	-4.73594500
H	4.77477500	2.62755000	1.00977200
H	5.44663300	-0.57760500	-1.13490800
H	3.91177700	2.61653100	-2.80055400
H	0.89967900	4.52490600	-3.69764700
H	4.89814900	-3.73680900	0.65183600
H	3.71545100	1.93358700	4.45731000
H	1.34205500	-0.81031600	5.02977000
H	1.99947400	-3.99920800	2.88675800
H	-1.68816300	-2.90747100	3.70736200
H	0.71222200	2.81196400	5.13813900
H	-2.00749500	4.31675400	-1.45061900
H	-1.14913200	4.32336000	2.34733700
H	-4.08444000	2.29630700	1.05556000
H	2.44417900	4.57815000	3.06688300
H	-1.34260200	1.63075900	4.78463000
H	-3.05259900	0.43645100	3.98723100
H	2.47233300	-5.47566500	-0.44604600
H	-1.92645900	-4.67839700	0.53410600
H	-4.65756500	0.24305100	-2.07263400
H	-3.25546500	1.47968100	-3.35044600
H	1.54955700	5.03508600	-1.44864000
H	2.04160800	5.01214700	0.74478100
H	4.52357200	-0.07336200	3.42881300
H	4.89508100	-1.90822900	2.19953800
H	3.49770900	-1.90055400	-3.90717400
H	2.62466400	-0.07329500	-4.88964700
F	-5.35693400	-1.24027000	-0.14870800
O	-8.04589200	-0.59476700	0.36730300
H	-7.18670900	-1.05365400	0.38657000
H	-8.49099100	-0.96172800	-0.41165900
O	-6.41809800	1.58810400	-0.23947900
H	-7.13567300	0.95789600	-0.00357700
H	-6.69784400	1.97851200	-1.08048100

Si-F-3H_2O

Si	-1.50753900	-2.17455500	-3.97771600
Si	-4.14909100	-2.57654500	-1.40846100
Si	-1.89516400	-3.15069400	-1.85499000
Si	-3.81069100	0.62375500	-3.24952200
Si	-1.54066300	0.18385600	-3.76432200
Si	-0.40372500	-2.36034200	-0.17138500
Si	-3.12017200	-2.77733000	2.68585800
Si	1.83893400	-2.91340800	-0.75877800

Si	-0.94626000	-3.33656600	1.93311200
Si	2.53630200	-1.91284300	-2.79015200
Si	-0.03836300	1.00464400	-2.10520100
Si	-2.83787300	0.58191600	0.59119000
Si	-4.30884600	-0.23403200	-1.09829700
Si	2.21167300	0.42944300	-2.64196800
Si	-0.59748800	0.01322700	-0.00723200
Si	-2.41498500	4.06685100	-1.25012000
Si	-0.25109100	3.37169400	-1.91606000
Si	0.46791900	-2.54823000	3.65977500
Si	3.43901500	-2.06426300	0.76462600
Si	0.90079300	0.81855600	1.66456000
Si	-1.88362500	0.23288700	4.42677000
Si	-3.35701500	-0.42098500	2.69149300
Si	3.14505700	0.26273100	1.08257500
Si	0.34725000	-0.18603000	3.75294500
Si	3.81412000	1.10848800	-1.02689100
Si	1.14043300	4.28415100	-0.23151500
Si	-1.51195400	3.88325000	2.33516100
Si	-3.01044600	2.95427200	0.75406600
Si	0.69214600	3.18821000	1.81903100
H	3.99751800	-2.16707600	-2.95265400
H	5.08412500	0.44789300	-1.43930800
H	-0.26939000	-2.68105000	-4.62537000
H	-1.76506800	-4.63782200	-1.95184000
H	-4.94995000	-2.92653800	-2.61939400
H	-3.23767000	-3.24274300	4.10018700
H	-0.81734300	-4.82287500	1.82277100
H	1.97163600	-4.40121800	-0.83937700
H	-0.02664300	-3.09565000	4.95768700
H	-4.41466700	3.31090600	1.12702900
H	-5.71375400	0.12508200	-0.73023200
H	-4.76015900	-0.06130400	3.06541800
H	-2.16711500	-0.63908600	5.60581300
H	-4.64760500	-0.12510300	-4.23412100
H	-2.34198000	5.52709700	-0.94490800
H	0.08813000	3.99270300	-3.23421200
H	-1.19846300	0.80875900	-5.07976400
H	2.55133800	1.04240700	-3.96488900
H	0.76871400	5.72112800	-0.06570000
H	1.29150400	0.31802900	4.79804300
H	1.63352000	3.68447200	2.87058300
H	4.03823900	0.73943400	2.17720400
H	-1.56280200	5.36817600	2.18376700
H	2.58118300	4.24382400	-0.59500500
H	4.02481800	2.57679800	-1.03795700
H	-2.65132900	-2.55920400	-4.85781800
H	1.85534800	-2.51638800	-3.96531800
H	3.55866200	-2.84470500	2.02417700
H	1.86703700	-3.02525000	3.48825500
H	-2.09172900	1.63848400	4.86337600
H	-1.89384100	3.57391300	3.73821100
H	-3.42888800	3.89594700	-2.32364200
H	-4.16066500	2.06211900	-3.38455100
H	-4.71903500	-3.34457500	-0.27039100
H	-4.18514900	-3.46507300	1.90974200
F	4.90269100	-2.24935600	0.01359200
O	8.10320500	0.76739000	-1.26672700
H	7.57645400	0.57166700	-2.05630000
H	8.06208200	-0.06290600	-0.72673500
O	7.48954000	-1.05312100	0.67674600
H	7.11094400	-0.23232700	1.05968200
H	6.70956600	-1.57234900	0.41727500
O	6.51665600	1.56817200	0.78534900
H	7.08003400	1.53224200	-0.03018900
H	6.87186900	2.29735500	1.31543100

Si-F-4H_2O

Si	-1.79182400	-2.52851100	-3.73456200
Si	-4.25438500	-2.82189900	-0.98285100
Si	-2.00733300	-3.34250400	-1.52097600
Si	-4.15471900	0.22927100	-3.09144500
Si	-1.89988700	-0.16247200	-3.70478300
Si	-0.46118400	-2.35973600	0.00365300
Si	-2.98861300	-2.64935200	3.04931800
Si	1.77182900	-2.86039300	-0.65196000
Si	-0.84261200	-3.18366600	2.20518200
Si	2.29614400	-2.01345700	-2.80251200
Si	-0.34347200	0.84847800	-2.20772000
Si	-2.97372000	0.53681500	0.67697400
Si	-4.49877100	-0.46976400	-0.85395600
Si	1.90089700	0.32245900	-2.82328400
Si	-0.74947100	0.00920500	-0.01054200
Si	-2.81053900	3.87340200	-1.45291500
Si	-0.65988200	3.21175300	-2.19340200
Si	0.65471200	-2.20462400	3.75403300
Si	3.45000400	-1.82802500	0.66686900
Si	0.81078400	1.00050300	1.49326900
Si	-1.78108900	0.52796600	4.46427400
Si	-3.32654700	-0.31173500	2.87778200
Si	3.04691600	0.49916600	0.83539800
Si	0.42184000	0.14946600	3.68361400
Si	3.55694600	1.20616100	-1.36837800
Si	0.77363600	4.32098800	-0.66989300
Si	-1.69512800	4.01111800	2.07739600
Si	-3.24125600	2.90537600	0.66512800
Si	0.50309100	3.36447800	1.47940100
H	3.74656200	-2.24436500	-3.05930700
H	4.84511800	0.59943700	-1.79384100
H	-0.58436100	-3.04984900	-4.42663000
H	-1.82099000	-4.82689900	-1.50860200
H	-5.11271300	-3.30393900	-2.10608700
H	-3.00209200	-2.99711800	4.50207200
H	-0.65710000	-4.66830000	2.20472700
H	1.96173400	-4.34471900	-0.62575500
H	0.30488800	-2.67966500	5.12577800
H	-4.63566900	3.23779200	1.09399000
H	-5.89653600	-0.13630800	-0.43685800
H	-4.71863900	0.02538700	3.31027200
H	-1.95697800	-0.26426700	5.71863000
H	-5.01283600	-0.62838300	-3.96283400
H	-2.78400400	5.35561500	-1.26877500
H	-0.42611300	3.74047700	-3.57341600
H	-1.66383300	0.36508500	-5.08478000
H	2.13200000	0.83644100	-4.21003000
H	0.32855900	5.74464100	-0.58576300
H	1.40100500	0.77150200	4.62898600
H	1.47999000	3.98313800	2.42972700
H	3.94345700	1.12311400	1.84737700
H	-1.82051600	5.47766300	1.82285900
H	2.19127000	4.33424500	-1.11666500
H	3.66403200	2.68201100	-1.49018300
H	-2.97847100	-3.01539200	-4.50044700
H	1.54570500	-2.72198200	-3.87251700
H	3.72688000	-2.51621200	1.95430800
H	2.05907500	-2.62292100	3.49131900
H	-2.02387900	1.95257600	4.81363200
H	-1.98247400	3.79472100	3.52004100
H	-3.87867400	3.57849500	-2.44393900
H	-4.57646800	1.63675200	-3.31781100
H	-4.72093100	-3.51169700	0.24893300
H	-4.06702000	-3.44206500	2.40203200
F	4.80903300	-2.03692000	-0.24873700
O	7.83210200	0.81897200	-1.66428700
H	7.37331200	1.40185900	-1.01033100
H	8.74667300	1.13740300	-1.68887600
O	7.63690900	-1.49566800	-0.20882400

H	6.81521700	-1.91712900	-0.51057700
H	7.76168300	-0.72822200	-0.82559900
O	6.56151500	-0.20714100	1.85835400
H	7.01470500	-0.75588100	1.15020300
H	7.09405700	-0.32521300	2.65856500
O	6.46105100	2.03011000	0.36103700
H	6.58905700	2.85794900	0.84529500
H	6.49226900	1.29982700	1.03572700

Si-F-5H_2O

Si	-1.08638300	-0.22193100	4.61051400
Si	-4.24053800	0.89195400	3.01542900
Si	-1.99734500	1.57000300	3.35871200
Si	-3.26752500	-2.68081800	2.90647400
Si	-0.98347300	-2.15053900	3.24030000
Si	-0.83883500	1.96536900	1.31298700
Si	-4.12903800	3.21646100	-0.50793400
Si	1.42740500	2.54968000	1.76853400
Si	-1.89662800	3.72218600	0.09865800
Si	2.61666900	0.83021800	2.88557600
Si	0.19659100	-1.78840200	1.20122700
Si	-3.13466500	-0.62253700	-0.47624800
Si	-4.27568500	-0.99447800	1.58381800
Si	2.45839600	-1.17545400	1.63384400
Si	-0.87148300	-0.02575900	-0.00297300
Si	-2.04684500	-4.42592100	-0.73879900
Si	0.14426900	-3.76457400	-0.13064300
Si	-0.84342400	4.13401800	-1.98108000
Si	2.70904000	2.84420200	-0.19905000
Si	0.29579400	0.35657200	-2.04879000
Si	-3.05421300	1.69067200	-3.69727100
Si	-4.17033400	1.15765800	-1.67767500
Si	2.56118800	0.92738200	-1.57827500
Si	-0.77358200	2.12595100	-3.23310900
Si	3.74368500	-0.67580800	-0.29311800
Si	1.22631400	-3.47844000	-2.21690500
Si	-1.94640000	-2.38463800	-3.82102200
Si	-3.14555500	-2.61123100	-1.79160700
Si	0.25122900	-1.64113300	-3.34797500
H	4.05687300	1.23285100	2.92930500
H	4.95108800	0.01330800	0.21320400
H	0.22288800	0.11800500	5.22716400
H	-1.97043100	2.82250200	4.17645700
H	-4.78553500	0.46267900	4.33809500
H	-4.58663300	4.27906800	-1.45262100
H	-1.86990600	4.96738000	0.92751800
H	1.45649700	3.80708400	2.57873100
H	-1.67341100	5.12252200	-2.73181000
H	-4.56376900	-2.98526200	-2.08697000
H	-5.69402000	-1.36932400	1.29020400
H	-5.58774300	0.78183100	-1.97434000
H	-3.65633700	2.95293300	-4.22192200
H	-3.93587200	-2.66177700	4.24210100
H	-1.92290100	-5.51831900	-1.74998500
H	0.80549600	-4.87253700	0.62681500
H	-0.32023900	-3.26017800	3.99351000
H	3.10014800	-2.27756400	2.41384400
H	0.97132100	-4.70199400	-3.03455100
H	-0.03818300	2.36643900	-4.51362400
H	0.98194700	-1.39452600	-4.62993500
H	3.24964900	1.20577100	-2.87504400
H	-1.84157300	-3.74321300	-4.43275400
H	2.69915800	-3.33909600	-2.07736400
H	4.11318300	-1.87747700	-1.07565000
H	-2.03416800	-0.51159000	5.72797400
H	2.18086700	0.68620200	4.29953600
H	2.44385800	4.12878900	-0.89929200
H	0.50652900	4.73650100	-1.81248800

H	-3.23433200	0.65280700	-4.74618800
H	-2.64373300	-1.51614200	-4.80582700
H	-2.81814800	-4.97829400	0.40584500
H	-3.46211300	-4.04177500	2.34088100
H	-5.10364500	1.99939800	2.52695800
H	-5.05471800	3.23888900	0.65499000
F	4.28253400	2.96581000	0.29995100
O	6.45735800	-2.07708500	1.25932800
H	6.92419900	-2.09780600	0.37705700
H	6.76645800	-2.86444400	1.73140700
O	6.97086600	1.92493300	-0.22898200
H	6.15462500	2.43003100	-0.07827400
H	7.08824700	1.40519000	0.60948000
O	6.42864100	0.15577000	-2.15366200
H	6.63540600	0.85416600	-1.46392900
H	6.72461100	0.52697700	-2.99807600
O	7.80125100	-1.91596400	-1.07490600
H	8.63376900	-1.47553200	-0.84524200
H	7.29483000	-1.22338000	-1.57871700
O	7.09786300	0.44204300	2.07877200
H	6.34599900	0.72403100	2.62178100
H	6.89831400	-0.50427900	1.85738800

Si-OH-vac

Si	0.09092600	4.32430300	-1.64735500
Si	2.35731700	3.83704700	1.23191400
Si	0.05691500	3.82397100	0.66779400
Si	3.29850300	2.57105900	-2.12756600
Si	1.03497000	2.49760400	-2.82348500
Si	-1.01063700	1.75182500	1.17109800
Si	1.33760500	1.13897500	4.30795300
Si	-3.29269800	1.83262400	0.48151300
Si	-0.88545600	1.31716700	3.51083800
Si	-3.53074400	2.16843400	-1.85107000
Si	-0.02134200	0.41210300	-2.35097600
Si	2.39705500	-0.07802900	0.67956100
Si	3.42606700	2.01065900	0.16976400
Si	-2.31896300	0.48389700	-2.99364000
Si	0.10820000	-0.00113000	-0.00235900
Si	3.37267700	-1.57719500	-2.85424200
Si	1.10575000	-1.34601500	-3.50280300
Si	-1.83222500	-0.77033500	4.10444100
Si	-4.44208200	-0.20265000	0.83267300
Si	-0.93443500	-2.09024400	0.49752800
Si	1.42438300	-2.49804300	3.66270400
Si	2.49440300	-0.48360600	3.02709600
Si	-3.22032200	-1.97725800	-0.16745000
Si	-0.79746600	-2.48615500	2.84328200
Si	-3.47158200	-1.51991800	-2.47782700
Si	0.21765300	-3.49168200	-3.03643500
Si	2.49022300	-3.95470500	-0.15312400
Si	3.48971600	-1.83650700	-0.50285000
Si	0.18710900	-3.82595000	-0.69186800
H	-4.97018200	2.03610300	-2.21139300
H	-4.92143000	-1.30472600	-2.76001100
H	-1.23848400	4.73068800	-2.17330300
H	-0.64484300	4.91872000	1.40782500
H	2.95082200	5.09211300	0.68116100
H	1.27127400	0.63253400	5.71191100
H	-1.59435800	2.41076800	4.24592400
H	-3.97457200	2.93275700	1.23185700
H	-1.53039100	-1.01427600	5.54677800
H	4.92346100	-1.88642300	-0.07738500
H	4.86067100	1.95651200	0.59181200
H	3.92890300	-0.52488100	3.45064100
H	1.35260600	-2.51753300	5.15458400
H	3.76438500	3.98305900	-2.27112900
H	3.88892000	-2.83610600	-3.47075800

H	1.03230500	-1.08570300	-4.97453800
H	0.95701200	2.75663400	-4.29517100
H	-2.38956700	0.73316100	-4.46772400
H	1.15711600	-4.49836200	-3.61561800
H	-1.45265000	-3.79572400	3.15186400
H	-0.47445100	-5.13066400	-0.37685000
H	-3.87829600	-3.28586900	0.15168300
H	3.12389200	-4.91257000	-1.10814400
H	-1.10781500	-3.71981800	-3.66934100
H	-3.03314200	-2.65621500	-3.33073500
H	1.00738200	5.48939200	-1.83385600
H	-3.09493000	3.52976400	-2.25968300
H	-4.72464300	-0.48206600	2.27040500
H	-3.31253300	-0.78003900	3.95862200
H	2.17983200	-3.70910600	3.24724500
H	2.73015300	-4.48228900	1.21602700
H	4.22835600	-0.46748300	-3.35063400
H	4.18990000	1.73189000	-2.97073900
H	2.58702000	3.85367900	2.70056400
H	2.04037800	2.44838700	4.35153400
O	-5.89376900	0.01841200	0.00457000
H	-6.52323700	-0.71703000	0.03849900

Si-OH-1H_2O

Si	-0.82769800	4.38381300	-0.98525000
Si	1.47466200	4.03289900	1.88789000
Si	-0.74519000	3.53922000	1.22614000
Si	2.74210300	3.57771600	-1.56277800
Si	0.57408000	3.06790900	-2.36766500
Si	-1.27248500	1.21677400	1.36142100
Si	1.15158800	0.71991900	4.47125600
Si	-3.51602200	0.87671700	0.61067600
Si	-1.04309600	0.47248600	3.61559000
Si	-3.83335100	1.48645800	-1.65702300
Si	0.05378800	0.74361000	-2.26215500
Si	2.49781700	0.37764300	0.76026300
Si	2.97973900	2.70850500	0.62693900
Si	-2.19287300	0.38887900	-2.97235500
Si	0.26534600	0.00579900	-0.00178300
Si	3.82473600	-0.26839800	-2.91979900
Si	1.57329600	-0.49153800	-3.62131500
Si	-1.43506700	-1.84972600	3.86576000
Si	-4.08273900	-1.42071600	0.62651100
Si	-0.23453400	-2.32482000	0.13220900
Si	2.13882400	-2.64768800	3.29346500
Si	2.68113400	-0.35911600	3.01998700
Si	-2.47478700	-2.65104500	-0.61269200
Si	-0.01566900	-3.04375000	2.39430400
Si	-2.82801400	-1.88837600	-2.82792600
Si	1.22831000	-2.83258100	-3.52251300
Si	3.54175600	-3.17880400	-0.65139700
Si	3.99292300	-0.85349300	-0.63057800
Si	1.27967200	-3.53000400	-1.25975600
H	-5.14447300	0.97896700	-2.13591500
H	-4.29041400	-1.98364000	-3.11581000
H	-2.21374800	4.48965700	-1.51067300
H	-1.70166100	4.30080800	2.08841800
H	1.73892600	5.46162800	1.54171500
H	1.20302100	0.00883000	5.78389700
H	-2.00257400	1.22988000	4.47860500
H	-4.39507600	1.64867000	1.53507100
H	-1.06317900	-2.22744100	5.26209300
H	5.39380800	-0.62380800	-0.15795900
H	4.37662500	2.94003700	1.11031400
H	4.07856800	-0.11735900	3.49660400
H	2.06821600	-2.92319000	4.75977400
H	2.84905600	5.06453100	-1.46878400
H	4.63710700	-1.25464800	-3.69337200

H	1.44529400	-0.02916000	-5.03839900
H	0.44913700	3.52341900	-3.78730400
H	-2.31411700	0.83454000	-4.39595500
H	2.38067000	-3.48526000	-4.21336700
H	-0.33149900	-4.50445800	2.46924900
H	0.95823200	-4.98878700	-1.17442400
H	-2.81348400	-4.10901300	-0.53037400
H	4.39208400	-3.79118300	-1.71571900
H	-0.00502700	-3.26664600	-4.22966600
H	-2.13944900	-2.74945700	-3.82526600
H	-0.26125700	5.76562400	-0.95693400
H	-3.81039300	2.96005600	-1.84445000
H	-4.26665400	-1.97656100	1.99686500
H	-2.86665900	-2.21035900	3.68490700
H	3.17144600	-3.55589900	2.72902400
H	3.89931700	-3.84523300	0.62845300
H	4.38409800	1.07823200	-3.20876700
H	3.81903000	3.12108000	-2.48026700
H	1.68209400	3.89536900	3.35348800
H	1.51103800	2.13870600	4.73099000
O	-5.57986500	-1.50732600	-0.18084000
H	-5.88919000	-2.39394000	-0.41923000
O	-6.92960300	0.99707900	0.04252000
H	-6.64621700	0.08135000	-0.14173500
H	-7.18246300	0.98056100	0.97752200

Si-OH-2H_2O

Si	0.29415200	4.45515100	-1.24092700
Si	2.99314400	3.66617600	1.15669800
Si	0.63158600	3.74786200	0.99433800
Si	3.32427900	2.68980300	-2.40302000
Si	0.97631400	2.72954600	-2.71349300
Si	-0.40935600	1.66066000	1.48928500
Si	2.40830400	0.71421900	4.11403300
Si	-2.77139500	1.83540800	1.21060400
Si	0.09098600	1.01125700	3.72771400
Si	-3.37158400	2.39378800	-1.01279500
Si	-0.05731600	0.62989600	-2.25412200
Si	2.80281100	-0.18866300	0.27143900
Si	3.80749700	1.91716000	-0.21680000
Si	-2.42355300	0.81088400	-2.49753300
Si	0.43742300	0.00035900	-0.00359500
Si	3.12810800	-1.37793900	-3.49341800
Si	0.79556600	-1.03874200	-3.72882000
Si	-0.82697900	-1.09814400	4.28818300
Si	-3.94006900	-0.19515400	1.56304800
Si	-0.58663100	-2.10196500	0.47849600
Si	2.24473200	-2.85165200	3.15402100
Si	3.27266300	-0.81348600	2.52397800
Si	-2.94620300	-1.88595600	0.21873600
Si	-0.08004900	-2.71290900	2.72612100
Si	-3.54322900	-1.20799900	-1.97154300
Si	-0.08265400	-3.19733200	-3.30508400
Si	2.61757800	-3.97224200	-0.89840700
Si	3.62239600	-1.85276200	-1.22625200
Si	0.26368400	-3.74399500	-1.02660700
H	-4.85778900	2.30723000	-1.14982500
H	-5.01383800	-0.93145400	-1.99612000
H	-1.09413100	4.91970000	-1.49816200
H	0.10130000	4.78527200	1.93271200
H	3.52444100	4.95079700	0.61079600
H	2.56176700	0.08968400	5.46208200
H	-0.44239500	2.05145400	4.66130600
H	-3.28067600	2.89220200	2.13958500
H	-0.29967400	-1.48269400	5.63137200
H	5.10379000	-1.97008500	-1.05302600
H	5.28886000	1.79580900	-0.04619500
H	4.75487100	-0.92691100	2.69270800

H	2.42020900	-3.00453900	4.62933400
H	3.81075200	4.09859000	-2.49907900
H	3.48551300	-2.58713100	-4.29389900
H	0.48737400	-0.64099300	-5.13784400
H	0.66495100	3.12176200	-4.12338100
H	-2.73666400	1.19961100	-3.90839400
H	0.70807600	-4.16685800	-4.12095200
H	-0.72375500	-4.03035800	3.02280600
H	-0.38451300	-5.05757200	-0.72273300
H	-3.58374000	-3.21059000	0.50322800
H	3.04645100	-4.85151300	-2.02692500
H	-1.50255800	-3.33557000	-3.72272200
H	-3.30964700	-2.26412800	-2.99150400
H	1.19574900	5.62178500	-1.47955500
H	-3.00282900	3.78711900	-1.37633600
H	-3.96784200	-0.59130600	2.99867100
H	-2.30973800	-1.05882400	4.39073900
H	2.87515000	-4.03658700	2.51504900
H	3.06197800	-4.62838600	0.35921400
H	3.92980700	-0.24735100	-4.03046200
H	4.03016800	1.91249800	-3.45518000
H	3.46917000	3.55900300	2.56076300
H	3.15384800	1.99995900	4.14224700
O	-5.49057000	0.10918600	1.00952800
H	-6.05873700	-0.65492500	0.71323300
O	-7.63430600	1.28667700	-0.36634300
H	-6.87886600	1.25921300	0.25634200
H	-7.25755100	1.67796900	-1.16926500
O	-7.33531200	-1.43781600	-0.14356000
H	-7.69994900	-0.54871300	-0.37674500
H	-6.99873500	-1.79276200	-0.98078300

Si-OH-3H_2O

Si	-0.48582500	1.68515200	4.29904200
Si	-2.91733600	3.36663100	2.08115000
Si	-0.58680200	3.06068500	2.37338500
Si	-3.66301800	-0.00323000	3.42263300
Si	-1.36463400	-0.45126700	3.77646200
Si	0.47502300	2.09420600	0.46932400
Si	-2.05868000	3.86372800	-2.01613100
Si	2.79825100	1.77623500	0.91598100
Si	0.20838000	3.52186700	-1.42254900
Si	3.15697100	0.28217900	2.71979100
Si	-0.31153100	-1.45241800	1.88630500
Si	-2.87784900	0.31821100	-0.45025000
Si	-3.90395800	1.30396600	1.46269100
Si	2.01287700	-1.75236900	2.31840400
Si	-0.55485200	-0.00791900	0.00018900
Si	-3.62802900	-3.35092100	0.85359100
Si	-1.33152000	-3.55126900	1.39776300
Si	1.13577300	2.61691400	-3.40501600
Si	3.94511500	0.74520100	-0.87848000
Si	0.49372500	-0.99300400	-1.90543100
Si	-2.04342500	0.92514700	-4.27371400
Si	-3.10750200	1.76390100	-2.33174300
Si	2.81322300	-1.27424900	-1.42853900
Si	0.22491000	0.46222400	-3.77549500
Si	3.16476000	-2.65879000	0.46042200
Si	-0.43261500	-4.60228100	-0.52521800
Si	-2.86174900	-2.91788500	-2.74263800
Si	-3.87367700	-1.79734900	-0.91723500
Si	-0.53228300	-3.09835600	-2.35237300
H	4.61605100	-0.04019300	2.78824400
H	4.62580100	-2.65003400	0.78433200
H	0.87722700	1.61500000	4.88817600
H	0.05736700	4.37823100	2.66806100
H	-3.48632700	3.75458900	3.40643600
H	-2.07552700	4.57316700	-3.33019900

H	0.85072500	4.83891200	-1.12437500
H	3.39417500	3.10314400	1.24957300
H	0.70004700	3.48488800	-4.53935300
H	-5.32806100	-1.59331400	-1.20244600
H	-5.35769100	1.51103200	1.17642300
H	-4.56422300	1.96604600	-2.60624200
H	-2.06238100	2.00951000	-5.30040100
H	-4.13996300	0.81954200	4.57414000
H	-4.08563400	-4.68103600	0.35170900
H	-1.17220000	-4.45224500	2.58153100
H	-1.20520700	-1.36163300	4.95302600
H	2.18111800	-2.65890900	3.49726800
H	-1.31694000	-5.76022800	-0.85365900
H	0.88145700	-0.16334300	-4.96539600
H	0.12949700	-3.71522400	-3.54392300
H	3.47539200	-1.91383100	-2.61144300
H	-3.41731900	-4.30370000	-2.78090100
H	0.93100500	-5.14962800	-0.29905600
H	2.81554500	-4.08157800	0.20826700
H	-1.37690200	2.29402100	5.33141300
H	2.80396200	0.87618300	4.03571100
H	4.06046400	1.61525900	-2.07580500
H	2.62134600	2.61342500	-3.39542600
H	-2.75458900	-0.24174700	-4.85873900
H	-3.17650500	-2.28514500	-4.05025000
H	-4.46924200	-3.01672400	2.03262200
H	-4.49029200	-1.23792700	3.39662300
H	-3.23850800	4.46303700	1.13044100
H	-2.78477000	4.72511400	-1.04638500
O	5.48537700	0.34265500	-0.30643300
H	5.99678200	-0.31135400	-0.86392800
O	7.03751400	-1.30842200	1.45783800
H	6.43313400	-0.57620700	1.22362200
H	6.49571800	-1.90050400	2.00099100
O	6.99691000	-1.64075600	-1.26024100
H	7.21106600	-1.77966700	-0.30582700
H	6.51970300	-2.43808200	-1.53541100
O	6.20327600	3.10247400	-0.12132500
H	6.27731700	2.13022000	-0.14108700
H	6.25063100	3.32416400	0.82040800

Si-OH-4H_2O

Si	1.85700000	3.37585400	2.91468600
Si	3.86081700	0.29203700	3.32775200
Si	1.65360000	1.11324700	3.58279400
Si	4.51854400	2.53483200	0.46673100
Si	2.34515400	3.46441900	0.59852800
Si	0.02576500	-0.05483500	2.28965000
Si	2.01323100	-3.44124700	2.72974200
Si	-2.10601400	0.99172900	2.54696600
Si	-0.06793000	-2.33729900	2.98831900
Si	-2.18736600	3.21285600	1.73246000
Si	0.76196900	2.28491800	-0.73661300
Si	2.82284400	-0.98303600	-0.27301600
Si	4.40917200	0.23573600	1.02460000
Si	-1.39692300	3.25979200	-0.49928200
Si	0.66743800	0.01170600	-0.00945000
Si	3.49612100	1.28971200	-3.43753300
Si	1.41464800	2.34272300	-3.02842500
Si	-1.47015100	-3.74412300	1.69212900
Si	-3.72513600	-0.19103900	1.30146200
Si	-0.94821800	-1.17389900	-1.30932300
Si	1.13884300	-4.51695000	-0.72955300
Si	2.72574600	-3.24170700	0.47905500
Si	-3.09542200	-0.17886300	-0.99297700
Si	-0.97703600	-3.45537900	-0.60717600
Si	-3.10665400	2.09452800	-1.65034300
Si	-0.07839400	1.14334400	-4.42100200

Si	1.85206900	-1.97397000	-4.00070800
Si	3.42501200	-0.91580200	-2.57937900
Si	-0.29996600	-1.06834400	-3.60203800
H	-3.62715500	3.61832400	1.69756900
H	-4.38806400	2.71585400	-1.20943800
H	0.66294600	4.18436700	3.27662600
H	1.25960800	1.05189500	5.02480600
H	4.77534400	1.27570900	3.98141800
H	1.79151900	-4.89173900	3.00769900
H	-0.49244200	-2.39833300	4.42139500
H	-2.46841600	0.96778500	3.99807500
H	-1.10609200	-5.15037900	2.04266300
H	4.76414600	-1.56196200	-2.74653400
H	5.75761000	-0.38787400	0.84734900
H	4.07911400	-3.86243500	0.33159500
H	1.01026400	-5.84373000	-0.05555100
H	5.36345100	3.20547700	1.49983100
H	3.66824600	1.19320500	-4.91801800
H	1.47918800	3.76953300	-3.47426900
H	2.38363000	4.89197100	0.15214000
H	-1.33920900	4.67837700	-0.97302400
H	0.54186300	1.05466200	-5.77696400
H	-1.96204000	-4.21922400	-1.43251600
H	-1.30886200	-1.80531000	-4.42495000
H	-4.07964300	-0.93322400	-1.82053400
H	2.22930400	-1.63230100	-5.40514000
H	-1.38422000	1.83440900	-4.58388400
H	-3.03260600	2.26934900	-3.12427200
H	3.02073100	3.96236500	3.64436100
H	-1.49645400	4.18363200	2.62130600
H	-3.73302900	-1.60431800	1.78372700
H	-2.91922000	-3.61370300	2.01822400
H	1.57565400	-4.78060400	-2.12558500
H	1.88338200	-3.45629400	-3.89270000
H	4.64774700	2.07148800	-2.91520900
H	5.16398600	2.77922500	-0.84993900
H	4.07450200	-1.01446700	4.00385000
H	3.03835500	-2.96515000	3.69487700
O	-5.24223600	0.46077800	1.56676000
H	-5.96147800	-0.15007500	1.18793800
O	-6.57596700	2.64993100	0.48742300
H	-6.06798300	2.00589100	1.03306100
H	-5.93950600	3.35371500	0.29125700
O	-6.93193100	0.90734500	-1.59596700
H	-6.84244300	1.62564300	-0.91680500
H	-7.77714900	1.08317100	-2.03573200
O	-5.18783000	-3.29845500	-0.12655200
H	-4.67382900	-3.27059300	0.69693200
H	-5.56205800	-4.19242300	-0.15818500
O	-6.93444000	-1.07831800	0.28309100
H	-6.42785800	-1.87061900	0.00637500
H	-7.00424200	-0.49470100	-0.51464400

Si-OH-5H_2O

Si	-1.68555900	-2.58102000	-3.72294300
Si	-3.22557300	-3.89561900	-0.62492800
Si	-1.11150600	-3.50997000	-1.62144000
Si	-4.71475900	-0.96553300	-2.30948200
Si	-2.66934900	-0.45356600	-3.38705300
Si	0.27923600	-2.08210600	-0.31305400
Si	-1.28290600	-3.41998900	3.08004000
Si	2.33957200	-1.67523700	-1.44357800
Si	0.69053500	-3.08385100	1.81297100
Si	2.05479400	-0.62215600	-3.54431200
Si	-1.28211400	1.00445400	-2.11053800
Si	-2.89281900	-0.36233800	1.16137700
Si	-4.25669600	-1.81663900	-0.14758400
Si	0.78139900	1.35229400	-3.24736000

Si	-0.83182900	0.00410200	0.01102900
Si	-4.41085800	2.86749900	-0.56282000
Si	-2.38145300	3.09148800	-1.76264400
Si	1.97740900	-1.73165100	3.27199400
Si	3.79298900	-0.23411800	-0.24138500
Si	0.57615500	1.44457100	1.29371100
Si	-0.98757500	-0.04797900	4.61920000
Si	-2.43273400	-1.35934300	3.27657600
Si	2.63271600	1.80486700	0.12982000
Si	0.99475000	0.42051200	3.40908000
Si	2.25685200	2.73091600	-2.01905000
Si	-1.14195200	4.59179700	-0.41166800
Si	-2.66352700	3.28728100	2.67966200
Si	-3.98356800	1.73449700	1.47240500
Si	-0.55787100	3.51860300	1.61782200
H	3.40206200	-0.21479400	-4.04098800
H	3.55340400	2.74462700	-2.76623500
H	-0.53574100	-2.53508500	-4.66404300
H	-0.40729400	-4.81423800	-1.82502000
H	-4.07473600	-4.58967400	-1.63874300
H	-0.86465900	-3.84120900	4.45018500
H	1.38233000	-4.39401800	1.60222800
H	3.01350600	-3.00020600	-1.65478800
H	1.87931300	-2.34381800	4.63080700
H	-5.27195400	1.50422200	2.19707000
H	-5.54218600	-2.05422000	0.57983300
H	-3.72508500	-1.57670300	3.99814200
H	-0.60349100	-0.87254300	5.80349200
H	-5.37302500	-2.05517400	-3.09035600
H	-4.88597100	4.24173600	-0.22243600
H	-2.65133600	3.72061400	-3.09287300
H	-2.94544000	0.18430000	-4.71180900
H	0.50747900	1.97935200	-4.57752400
H	-2.04842300	5.72756500	-0.06673300
H	1.87333600	1.31987900	4.21859900
H	0.31344200	4.42509400	2.42812100
H	3.46701600	2.74392200	0.93737000
H	-3.34749700	4.61243500	2.59757600
H	0.02924900	5.17210600	-1.11919700
H	1.81204300	4.14792200	-1.95692500
H	-2.71947300	-3.46702400	-4.33630000
H	1.47047700	-1.53395900	-4.56257700
H	4.14113300	-0.84153000	1.07119000
H	3.42323200	-1.70561800	2.92159000
H	-1.64979300	1.17740200	5.13730400
H	-2.55169200	2.94376700	4.12141700
H	-5.48243900	2.22070500	-1.36467700
H	-5.65410700	0.18624000	-2.28910200
H	-3.14616900	-4.78789900	0.56108800
H	-2.14207600	-4.50247300	2.53334100
O	5.20535000	-0.02386200	-1.12839500
H	6.05833100	-0.00305300	-0.52295200
O	6.05476400	-2.76575000	-1.35025200
H	5.83060300	-1.83478900	-1.55808200
H	5.29560100	-3.27985300	-1.66358500
O	6.05980800	2.69435000	-1.31473700
H	5.76051700	1.78008900	-1.50732200
H	5.40280800	3.26506500	-1.73948100
O	6.79292100	-2.47591000	1.31668700
H	5.96123900	-2.53713000	1.81010900
H	6.55794600	-2.75372100	0.39928600
O	7.25596600	0.02804500	0.36557700
H	7.19407800	-0.79372600	0.91477400
H	7.13165500	0.82360100	0.94079300
O	6.65620200	2.48434400	1.36366800
H	6.40682500	2.72349400	0.43768200
H	7.46223500	2.99382200	1.53748800

Si-Si=O-vac

Si	0.77761000	3.96741200	-2.27079600
Si	2.17405500	3.95653300	1.19176100
Si	0.12645300	3.89595800	0.00394600
Si	3.89867200	2.11510500	-1.52079800
Si	1.91714100	1.96383500	-2.80994900
Si	-1.16204600	1.96100100	0.52297300
Si	0.14510200	1.81687100	4.25577000
Si	-3.18394200	1.96478600	-0.73845500
Si	-1.74060700	1.91920400	2.83149600
Si	-2.80836100	1.84833000	-3.07977800
Si	0.64162700	0.00925200	-2.32387500
Si	2.09909900	-0.00408600	1.30522500
Si	3.36129000	1.95006700	0.78086400
Si	-1.39321500	0.01229200	-3.56791700
Si	0.09838600	0.00023800	0.00002900
Si	3.90122700	-2.10155900	-1.53556600
Si	1.92022700	-1.93951600	-2.82439100
Si	-3.03044900	-0.01415300	3.27085900
Si	-4.46464000	-0.00083000	-0.35760700
Si	-1.15969300	-1.96600300	0.50846300
Si	0.14749700	-1.84801400	4.24284200
Si	1.50682700	-0.01242900	3.61762100
Si	-3.18205300	-1.96247900	-0.75206800
Si	-1.73767600	-1.94230600	2.81742300
Si	-2.80766400	-1.82786100	-3.09277400
Si	0.78158900	-3.94786200	-2.30120700
Si	2.17709600	-3.96396600	1.16236200
Si	3.36287200	-1.95346800	0.76705200
Si	0.13021800	-3.89556100	-0.02603400
H	-4.12084400	1.58276300	-3.73927300
H	-4.12053800	-1.55734800	-3.74950500
H	-0.37002100	4.23187400	-3.17814400
H	-0.68684200	5.10704500	0.33404000
H	2.98638700	5.08348000	0.64374700
H	-0.34026400	1.54728500	5.64239600
H	-2.54830400	3.13808000	3.14531400
H	-4.00159100	3.16737700	-0.40159200
H	-3.48934500	-0.01960000	4.69013200
H	4.62329200	-1.94831400	1.57294800
H	4.62207300	1.94046300	1.58616700
H	2.75903400	-0.01424000	4.43598000
H	-0.33867700	-1.58821400	5.63104900
H	4.47206200	3.47549500	-1.74716300
H	4.47301400	-3.46089100	-1.77211900
H	2.27010500	-1.92538900	-4.27883000
H	2.26641000	1.96097800	-4.26461100
H	-1.07826400	0.01723400	-5.03014900
H	1.74451300	-5.07574100	-2.47591100
H	-2.54377000	-3.16465700	3.12183600
H	-0.68228400	-5.10994000	0.29378100
H	-3.99830900	-3.16861500	-0.42450600
H	2.99068600	-5.08600500	0.60623500
H	-0.36642500	-4.20525300	-3.21005200
H	-2.29645400	-3.11376300	-3.63540200
H	1.74043200	5.09682400	-2.43574400
H	-2.29718500	3.13855700	-3.61202100
H	-4.25202800	-0.01202800	2.41137600
H	0.88232700	-3.14017000	4.26917500
H	1.98067300	-4.23771200	2.61064200
H	4.93472400	-1.11485600	-1.94562100
H	4.93054500	1.13021700	-1.93918600
H	1.97810200	4.21898400	2.64218400
H	0.87844400	3.10969800	4.29061000
O	-5.99433200	-0.00183400	-0.14654900

Si-Si=O-2H_2O

Si	-1.41767500	-2.92208400	-3.38733400
Si	-3.34030100	-3.42874200	-0.21431000

Si	-1.16797300	-3.61368100	-1.13733400
Si	-4.11218300	-0.56852800	-2.43592600
Si	-1.96022800	-0.61848300	-3.42669700
Si	0.41214800	-2.28761600	0.05222600
Si	-1.42048700	-2.76153200	3.53130500
Si	2.56782400	-2.50198400	-0.93280800
Si	0.59518400	-2.99378000	2.31638300
Si	2.64342300	-1.67866300	-3.15911900
Si	-0.38089000	0.73857500	-2.26641500
Si	-2.38558900	0.20300500	1.05073300
Si	-3.95097600	-1.14283600	-0.14252300
Si	1.79186400	0.53105800	-3.22823500
Si	-0.25104400	0.00703500	-0.00016500
Si	-3.16955100	3.35378200	-1.21876100
Si	-1.09176200	3.01394700	-2.30547200
Si	2.22118700	-1.63101100	3.35868100
Si	4.17505300	-1.10268600	0.11191300
Si	1.32657300	1.37121300	1.16145500
Si	-0.58039300	0.64174000	4.57298400
Si	-2.20250700	-0.53714600	3.31277900
Si	3.49863700	1.17135700	0.19559500
Si	1.47974100	0.61277800	3.41130600
Si	3.49486600	1.74227900	-2.10675400
Si	0.36703100	4.45302500	-1.12118300
Si	-1.52981200	3.93662700	2.05498700
Si	-3.06440900	2.48727300	0.98355200
Si	0.61140400	3.64212800	1.08931400
H	4.07646700	-1.62060700	-3.57392300
H	4.78601700	1.31400100	-2.71489800
H	-0.22141900	-3.24460100	-4.20957800
H	-0.71688300	-5.03893100	-1.09134000
H	-4.29073800	-4.12624300	-1.13068000
H	-1.11774400	-2.98816300	4.97611900
H	1.04902100	-4.41836000	2.34282000
H	3.03463900	-3.91876700	-0.88005100
H	2.56162400	-2.13242400	4.72093500
H	-4.40705500	2.60903100	1.63185200
H	-5.29489900	-1.00493100	0.49982800
H	-3.53886200	-0.41080600	3.97269700
H	-0.39658200	-0.09725400	5.85796100
H	-4.93030900	-1.62684700	-3.10035700
H	-3.37493200	4.82886400	-1.10693900
H	-1.19468600	3.45956400	-3.72973600
H	-2.05379400	-0.15037900	-4.84430200
H	1.74144500	0.97516200	-4.65583600
H	-0.28220200	5.79572000	-1.04800200
H	2.48643500	1.44508100	4.13885900
H	1.61330100	4.47457400	1.82389600
H	4.45002700	1.99252100	0.98871100
H	-1.96922200	5.33863400	1.78841000
H	1.67392100	4.63198000	-1.80690300
H	3.36965200	3.21094600	-2.29728700
H	-2.57015200	-3.67082600	-3.97112000
H	1.95089200	-2.60785400	-4.09009300
H	3.47923500	-1.69735200	2.54491100
H	-0.99599700	2.02662900	4.91877300
H	-1.51032400	3.75381900	3.53053300
H	-4.31680300	2.81097700	-1.99252700
H	-4.81159700	0.72472200	-2.65402500
H	-3.44110800	-4.09072000	1.11339100
H	-2.42183100	-3.78321900	3.12633300
O	5.63945400	-1.55810800	0.35379200
O	6.80213000	0.91503900	-0.31144100
H	6.64593000	0.02939100	0.08145200
H	7.17773400	0.71252600	-1.18113100

Si-Si=O-2H_2O

Si	1.80666300	-3.86335100	-2.02313400

Si	2.96893500	-0.76825400	-3.70845900
Si	1.00241200	-2.00584800	-3.25175100
Si	4.53815800	-1.82259500	-0.54017900
Si	2.64501000	-3.11196800	0.05891500
Si	-0.61669100	-0.71555700	-2.07130700
Si	0.52899400	2.67419700	-3.77371500
Si	-2.53747900	-2.04875100	-1.60479000
Si	-1.26263700	1.18574200	-3.35655800
Si	-2.00269000	-3.94260800	-0.28343200
Si	1.00816200	-1.88500000	1.28058100
Si	2.21226700	1.38415100	-0.44485700
Si	3.81310600	0.12073600	-1.68134400
Si	-0.88048200	-3.27696100	1.69331400
Si	0.30793600	0.01190900	0.00756800
Si	3.78531000	0.29530400	3.03460400
Si	1.91827500	-1.12682300	3.35064600
Si	-2.88413100	2.48261000	-2.22028200
Si	-4.16303700	-0.88645800	-0.29313300
Si	-1.32875800	1.26167500	1.23028000
Si	-0.20487000	4.51880400	-0.65821200
Si	1.51506200	3.27889500	-1.71006600
Si	-3.18527000	-0.15120800	1.74191700
Si	-2.03125400	3.11387900	-0.10279100
Si	-2.57512900	-2.13818800	2.88375800
Si	0.43999900	0.23177000	4.60934500
Si	1.62874000	3.31388000	2.94838500
Si	3.16355600	2.09264700	1.62266700
Si	-0.32996000	2.01814100	3.25910700
H	-3.31879700	-4.53931800	0.15627800
H	-3.76876400	-3.03700000	2.92528100
H	0.77982000	-4.92794600	-1.86343400
H	0.39580400	-2.48142900	-4.53402800
H	3.98932000	-1.72394200	-4.23463100
H	-0.05264600	3.91035600	-4.37738600
H	-1.82269900	0.70000800	-4.65622800
H	-3.17025800	-2.51826200	-2.87712300
H	-3.07917800	3.73707100	-3.00958700
H	4.36467300	2.93713500	1.33526300
H	4.99136900	0.99480000	-1.97466500
H	2.70489600	4.15255200	-1.95444800
H	-0.68955100	5.51657300	-1.65964300
H	5.34755100	-2.63614600	-1.49624500
H	4.14179900	0.87014300	4.36618300
H	2.32437500	-2.31682000	4.16175200
H	3.07219400	-4.28821600	0.87910000
H	-0.45509700	-4.50039700	2.44119500
H	1.23637600	0.81804500	5.72883800
H	-3.02015200	3.92820100	0.65774200
H	-1.33831200	2.81432800	4.02438100
H	-4.18463800	0.58441700	2.56470400
H	2.25092600	3.50951600	4.29223000
H	-0.66903800	-0.54294300	5.22549800
H	-2.17976200	-1.89140500	4.29478500
H	2.93886900	-4.46264200	-2.79065100
H	-1.33402300	-5.03174700	-1.04121900
H	-4.17701500	1.76351800	-2.16333500
H	0.29461700	5.29197300	0.51014700
H	1.34920800	4.66468100	2.39476100
H	4.98239900	-0.43558900	2.54148300
H	5.41221100	-1.51921100	0.62327100
H	2.75912900	0.26637700	-4.75470100
H	1.51196800	2.13536200	-4.75058600
O	-5.40021200	-0.18223800	-0.94146600
O	-5.23210300	-2.49274800	0.38690600
H	-6.06022600	-2.32053500	-0.10758400
H	-4.91522200	-3.39770000	0.19122100
O	-5.50744200	2.20812500	0.45334000
H	-5.62875700	1.40155100	-0.10144200
H	-5.78806200	2.93875800	-0.11649900

Si-Si=O-3H_2O

Si	-1.69350700	-4.45992000	0.28221900
Si	-2.76689700	-2.40944700	3.22082800
Si	-0.84176100	-3.23976800	2.12282200
Si	-4.57276100	-2.15245600	-0.01078200
Si	-2.70192800	-2.94380200	-1.22956200
Si	0.64099100	-1.50257700	1.45214600
Si	-0.26050200	0.77311300	4.56087500
Si	2.56278900	-2.40173400	0.36760900
Si	1.45673400	-0.27619800	3.32134300
Si	2.01807000	-3.54073200	-1.63469500
Si	-1.23157200	-1.19880300	-1.92158700
Si	-2.36777600	0.93329600	1.15923900
Si	-3.82896400	-0.83376900	1.81113400
Si	0.69410200	-2.11582200	-2.99162200
Si	-0.49682500	0.01266400	-0.00249000
Si	-4.23362700	1.36145200	-2.30277600
Si	-2.40225100	0.29449500	-3.36497700
Si	2.93759300	1.31593400	2.37025800
Si	3.95627300	-0.59212200	-0.28388100
Si	0.93389700	1.80110300	-0.71104300
Si	-0.02514100	3.79561400	2.58850300
Si	-1.57546400	2.08604900	3.09297300
Si	2.85527800	0.89018600	-1.77816600
Si	1.71224000	2.96465300	1.21226800
Si	2.28061900	-0.47880200	-3.62894200
Si	-1.08431300	2.12449800	-4.08097900
Si	-2.15131700	4.18097600	-1.11285100
Si	-3.51482000	2.42163600	-0.30835200
Si	-0.25092500	3.25368700	-2.17564300
H	3.25788500	-3.83478600	-2.39905300
H	3.51096100	-1.19732100	-4.07460300
H	-0.65589100	-5.30711100	-0.36274300
H	-0.09845500	-4.15965000	3.03837600
H	-3.71161700	-3.54662200	3.43193600
H	0.35894600	1.70903700	5.54677000
H	2.22654700	-1.20256300	4.20927900
H	3.26006700	-3.27154200	1.35767300
H	4.00050100	1.74616600	3.31290700
H	-4.69978900	2.99368600	0.40355600
H	-5.00922900	-0.24291900	2.51558300
H	-2.73933100	2.66145400	3.83563100
H	0.57944700	4.24970100	3.87753300
H	-5.26915800	-3.34405400	0.56035800
H	-4.71257400	2.43536300	-3.22416400
H	-2.89676900	-0.46282600	-4.55641200
H	-3.17446500	-3.68028200	-2.44293000
H	0.25653400	-2.86405400	-4.21117200
H	-1.97320400	3.06649300	-4.82443900
H	2.56592400	4.11919500	0.81349600
H	0.67540400	4.34949200	-2.59864500
H	3.77789000	1.97226700	-2.22381400
H	-2.93699900	4.93783900	-2.13261000
H	0.00607200	1.72152500	-5.00844000
H	1.82897400	0.36573400	-4.76743500
H	-2.76102000	-5.37404300	0.78726900
H	1.33755100	-4.82810000	-1.33217200
H	3.59853800	0.42051500	1.30401900
H	-0.64288000	4.99185600	1.95532400
H	-1.77025000	5.14505000	-0.04586500
H	-5.37918700	0.44166400	-2.07591800
H	-5.55802100	-1.44137100	-0.86673900
H	-2.44993500	-1.84596200	4.56024300
H	-1.04032500	-0.22657400	5.33724000
O	5.51588700	-0.76843400	-0.27443000
O	5.60093200	-3.56052500	-0.53110500
H	5.79526600	-2.60010200	-0.46267400

H	5.83447500	-3.90463900	0.34391700
O	7.15559100	1.34151500	0.07333200
H	7.40827400	1.57142000	-0.83382700
H	6.68321300	0.47351100	-0.02851400
O	4.85796800	2.64810400	0.67250600
H	5.05403600	3.55989200	0.93297600
H	5.74428200	2.22973300	0.49149600

Si-Si=O-4H_2O

Si	3.36119400	-3.38275500	1.60873700
Si	-0.04514200	-3.42780100	3.05311400
Si	1.92683700	-2.12020100	3.01055400
Si	0.54380000	-4.60904200	-0.45948900
Si	2.54273900	-3.35088800	-0.61468100
Si	1.55427400	0.09699100	2.21674900
Si	-2.17462300	0.21771500	3.63557400
Si	3.62156800	1.28346100	2.15936800
Si	-0.03274000	1.22984800	3.59310600
Si	5.20696300	0.29379200	0.70305900
Si	2.19567300	-1.14227100	-1.44239000
Si	-1.38815300	-1.22955400	0.05479300
Si	-1.00092400	-3.42551100	0.88812000
Si	4.26283700	0.04541800	-1.45586000
Si	0.66885100	-0.01273900	0.00433000
Si	-0.85209800	-2.26217200	-3.74084900
Si	1.26447600	-1.20977900	-3.63975100
Si	-0.54861800	3.41653100	2.84322000
Si	3.41731300	3.47814500	1.29667400
Si	0.34087300	2.20618300	-0.81987800
Si	-3.28259700	2.14532600	0.67491200
Si	-2.97053200	-0.09094300	1.42257200
Si	2.41795600	3.36940900	-0.84614600
Si	-1.22764800	3.33308000	0.57239900
Si	4.02677800	2.27998300	-2.19840100
Si	0.72470700	0.91411900	-4.53570000
Si	-2.69720100	0.95842700	-2.69187400
Si	-2.30461200	-1.30198500	-2.13994700
Si	-0.63067800	2.07707700	-2.98813100
H	6.35066600	1.24632800	0.57899700
H	5.33754500	2.96819000	-2.00388200
H	4.78020200	-2.95021400	1.70126700
H	2.51201400	-2.04911000	4.38531900
H	-3.09218800	1.16305400	4.33578700
H	0.49807000	1.30739000	4.98931800
H	4.18473700	1.33886600	3.54405100
H	-1.70127700	3.90691900	3.65403800
H	-3.57997100	-2.07624800	-2.11056600
H	-4.26467600	-0.82431700	1.43284700
H	-1.41625300	-1.99560800	-5.09818600
H	2.21920900	-1.91434100	-4.55033300
H	3.50992600	-4.05712300	-1.51103900
H	5.22756800	-0.67792200	-2.34122000
H	-0.07133400	0.67841800	-5.77744300
H	-1.48262000	4.70764000	0.04881400
H	-0.88376100	3.46668500	-3.48056900
H	2.17489300	4.75161800	-1.36303100
H	-3.62993300	1.19173600	-3.82587000
H	1.91369900	1.71881700	-4.92287600
H	3.69280800	2.36608200	-3.64488700
H	3.30365600	-4.79860100	2.08092200
H	5.75671900	-0.98020500	1.23610400
H	2.68209400	4.38898500	2.21344100
H	0.56947400	4.37819800	3.03046200
H	-3.27290200	1.61882100	-1.45995200
H	-0.78837500	-3.73897400	-3.57697500
H	-1.00939500	-2.97943400	4.09208200
H	4.79513000	4.03051700	1.13463000
H	0.34341800	-4.83123300	3.38296300

H	-2.30970000	-4.15161400	0.91046800
H	-2.19292600	-1.06424300	4.38804600
H	-0.02561600	-4.94516400	-1.79158900
H	0.86648000	-5.89731700	0.22290700
O	-4.64535200	2.88898300	0.72049200
O	-5.71378800	-0.00312100	-1.89708400
H	-6.15116400	0.62529300	-1.22659800
H	-6.22021000	0.11610100	-2.71510200
O	-6.87199600	1.44588000	-0.05116000
H	-6.19581900	2.07832800	0.28713500
H	-6.97107200	0.77037900	0.66349600
O	-6.97742300	-0.72982400	1.65911300
H	-7.88693900	-0.94235700	1.91693200
H	-6.75941800	-1.37878700	0.94087700
O	-6.30958800	-2.25954100	-0.50244000
H	-6.10085700	-1.50465500	-1.11439200
H	-5.46449800	-2.71804800	-0.38636500

Si-Si=O-5H_2O

Si	1.72059100	4.50723800	-0.53903100
Si	3.25647800	3.04498800	2.46726700
Si	1.13257000	3.54647600	1.54508700
Si	4.68328100	2.35159500	-0.88399400
Si	2.62081800	2.82652800	-1.94682300
Si	-0.29521300	1.64592500	1.33750300
Si	1.26251200	0.01284000	4.58986700
Si	-2.33136100	2.28240300	0.27052000
Si	-0.71594100	0.71675200	3.49437200
Si	-2.00453400	3.13392700	-1.91775500
Si	1.22626800	0.90455600	-2.17636900
Si	2.86820400	-0.61666300	1.02084400
Si	4.25772500	1.31214600	1.20135200
Si	-0.84928500	1.50253500	-3.18819400
Si	0.80039700	0.00210400	-0.00564000
Si	4.36238300	-1.50939100	-2.53188500
Si	2.33504300	-0.74793600	-3.49156100
Si	-1.98319200	-1.28438100	3.46556900
Si	-3.83258200	0.52541600	-0.26354700
Si	-0.60207800	-1.92234900	-0.20122500
Si	1.00473900	-3.39264400	3.12699500
Si	2.42805000	-1.50138700	3.18982700
Si	-2.66085600	-1.29623800	-1.22948500
Si	-0.98428800	-2.82570900	1.97240900
Si	-2.32773300	-0.34019800	-3.37515400
Si	1.10067700	-2.75848600	-3.70799700
Si	2.61182600	-4.19550100	-0.67351400
Si	3.94018300	-2.26502900	-0.32755200
Si	0.51067400	-3.54445200	-1.55201700
H	-3.34137600	3.36490400	-2.53346700
H	-3.63587500	0.15799700	-3.88282700
H	0.60707400	5.26603300	-1.16559700
H	0.44965100	4.57285400	2.39370500
H	4.10560400	4.26420200	2.31316500
H	0.85233000	-0.73370300	5.81692400
H	-1.41422200	1.73928600	4.33564400
H	-3.02647700	3.30936000	1.11478400
H	-1.87706100	-1.87555100	4.83416600
H	5.22970100	-2.65427600	0.32411000
H	5.55290500	0.91417000	1.83625500
H	3.72720300	-1.87361700	3.83223000
H	0.62386900	-3.71929200	4.53396400
H	5.35713900	3.65526900	-0.60567700
H	4.82162100	-2.68525100	-3.33032200
H	2.60912100	-0.18056600	-4.84870400
H	2.88118500	3.40071800	-3.30380500
H	-0.56494100	2.05003800	-4.55176100
H	2.01902600	-3.77437900	-4.30520100
H	-1.85289400	-4.03744200	1.85011700

H	-0.36821500	-4.74829500	-1.68199800
H	-3.54101300	-2.49648900	-1.34606500
H	3.29383500	-5.02558700	-1.71127600
H	-0.06162100	-2.63385500	-4.62517300
H	-1.81880100	-1.33247300	-4.35814600
H	2.81684500	5.48727900	-0.27449900
H	-1.28550400	4.43520900	-1.92963900
H	-3.42647100	-1.06438700	3.20400700
H	1.68140800	-4.59392100	2.57152100
H	2.49455700	-5.03704300	0.54623400
H	5.44806900	-0.49556700	-2.58957700
H	5.60608300	1.56021600	-1.73935700
H	3.20331700	2.73551600	3.92027200
H	2.11289200	1.14677700	5.03786300
O	-5.07087500	1.01041800	-1.15513000
O	-8.77040100	0.25962200	0.04514800
H	-9.38365800	0.76913400	-0.50530200
H	-8.13135800	0.92159900	0.39651300
O	-4.63921800	0.00462900	1.30359500
H	-5.14877200	-0.95772500	1.16553000
H	-5.36982500	0.68071700	1.43354100
O	-6.57575200	1.78764400	0.75838200
H	-6.53071600	2.73356200	0.96813800
H	-6.07073200	1.65262800	-0.13209900
O	-6.83178600	-1.11440300	-1.36451400
H	-7.63809800	-0.67407900	-0.99957500
H	-6.19955700	-0.36366700	-1.51798900
O	-5.80339300	-2.10794600	0.77257200
H	-6.24699000	-1.82949600	-0.12166700
H	-6.52283400	-2.36143400	1.37242400

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