

Calcium Silicate Hydrate (CSH)

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Investigating the bonding, polarity, IMFs, and properties of CaH_2SiO_4

Chemical Bonding

Polar

In a polar covalent bond, valence electrons are shared unequally between atoms due to a high electronegativity (EN) difference (between 0.5 and 1.7). The electron density shifts towards the more electronegative atom, as it has a stronger coulombic attraction that pulls the bonding electrons closer.

This gives it a partial negative charge and the less electronegative one a partial positive charge (see fig. 1). The opposite partial charges strengthen the attraction between the atoms, adding to the existing electrostatic attractions between the nuclei and shared electrons.

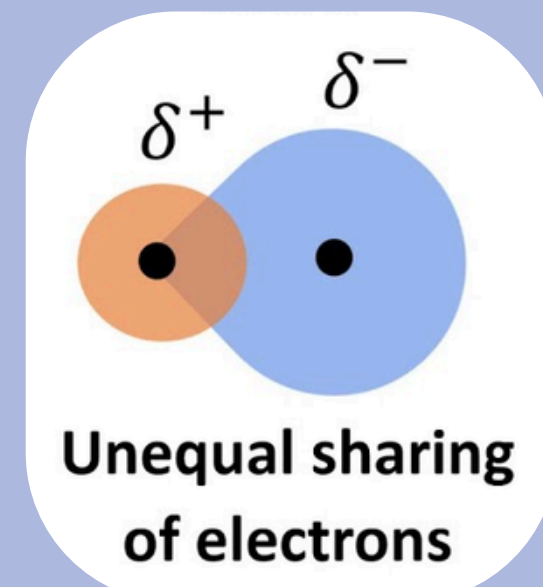


Fig. 1 Polar Bonding

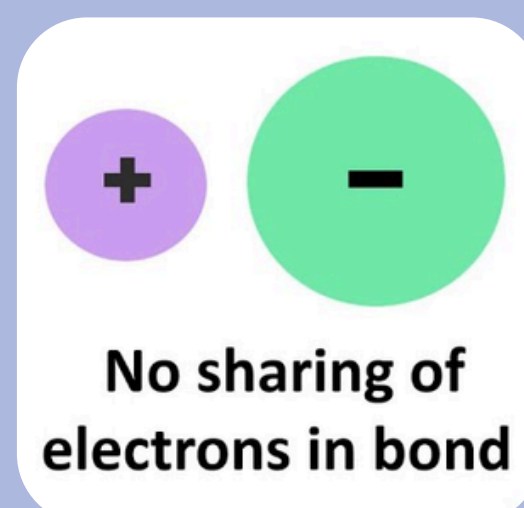


Fig. 2 Nonpolar Bonding

Ionic

An ionic bond is a complete transfer of valence electrons from a metal to a nonmetal, creating opposite charges on the atoms that electrostatically hold them together (as shown in fig. 2). Like polar bonds, they form to fill the valence shells of bonding atoms, leading to the most stable configuration. These bonds are far stronger than covalent ones, as the higher opposite charges on the atoms create stronger electrostatic attraction between them.

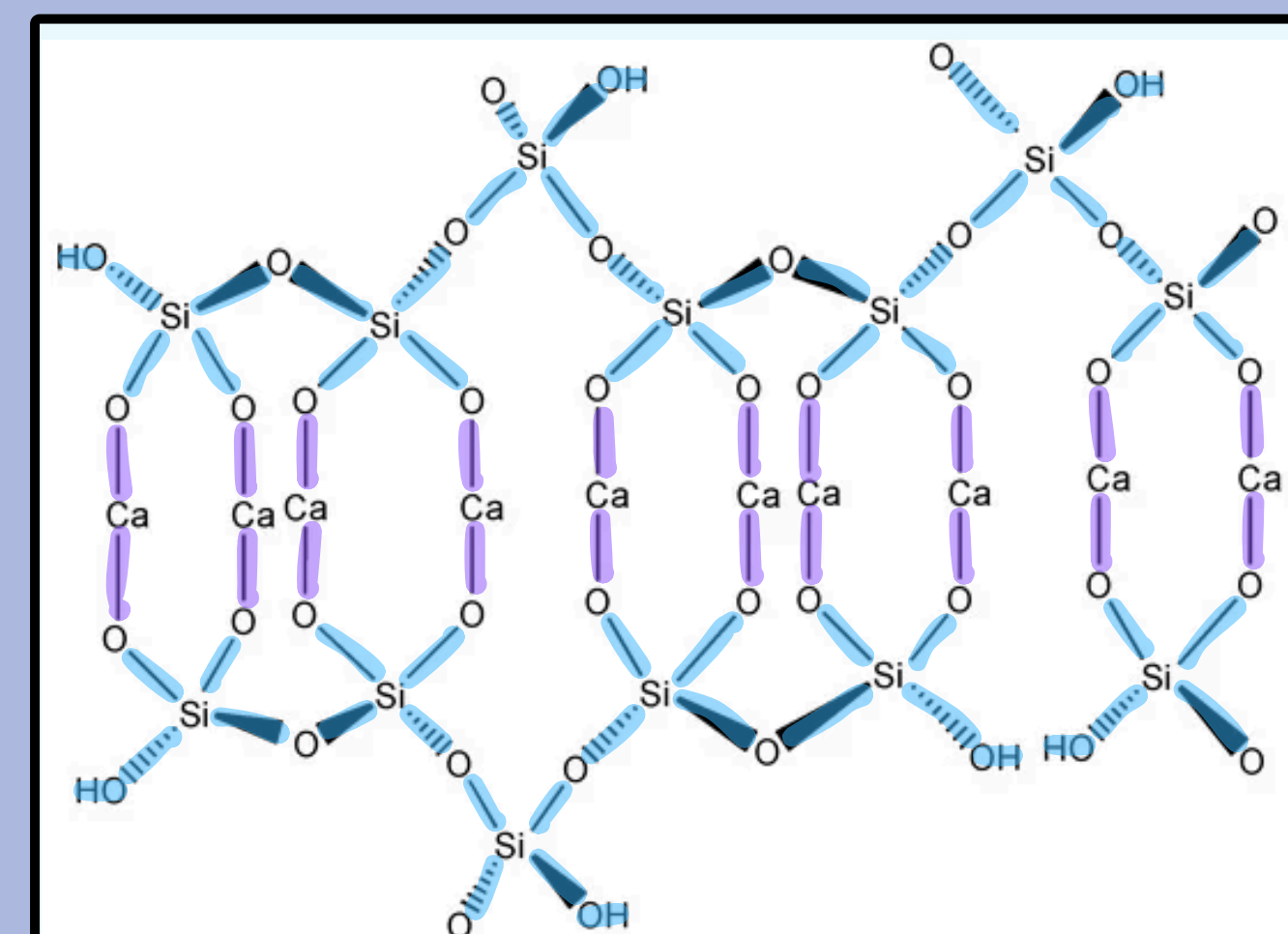


Fig. 3 CSH molecular structure

In fig 3., Ca gains a 2+ charge because it has 2 valence electrons it must get rid of for a full valence shell. These 2 valence electrons are donated to the H_2SiO_4 group, giving it a 2- charge.

VSEPR and Polarity

Bent ($<120^\circ$)

Polar

In fig. 5, highly polar bonds exist between Si-O and O-H. O has 2 nonbonding and 2 bonding domains. This creates a bent structure, since VSEPR theory states that molecules configure themselves to minimize electron-electron repulsions. Lone pairs will repel each other and bonding domains, bending the structure. This asymmetrical structure results in bond dipoles that do not sum to 0. Instead, they create a stronger molecular dipole (shown in pink) pointing from the O (electron density is highest near the O). The existence of a molecular dipole means it is highly polar, with an uneven electron density around the center.

Center =

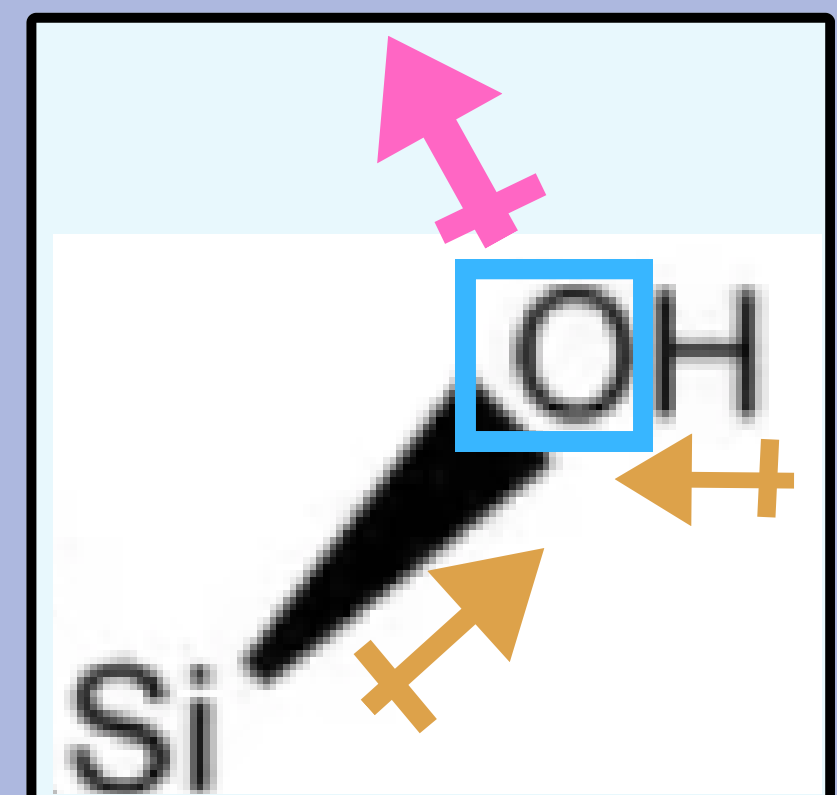


Fig. 5 Bent center

Tetrahedral (109.5°)

Nonpolar

As stated earlier, all the Si-O bonds surrounding the center in fig. 4 are polar. Consequently, there exist bond dipoles going from the Si to each O, as shown with the orange in fig. 4. These indicate the direction of electron density. With 4 total bonding domains, the center has a symmetrical tetrahedral structure to minimize repulsions. However, since all of these dipoles are of the same magnitude (with the same Si-O bond occurring 4 times) and go in opposite directions, they sum to 0. If the bond dipoles sum to 0, then the center as a whole is nonpolar, because the electrons are evenly distributed around the center.

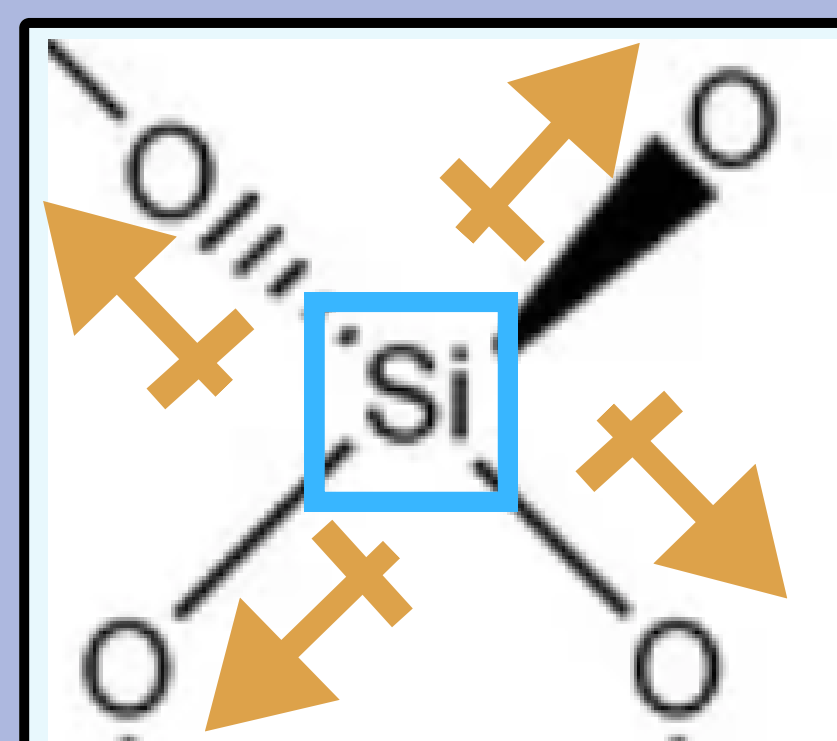


Fig. 4 Tetrahedral center

Intermolecular Forces

London Dispersion Forces (LDFs)

LDFs are temporary attractive forces that result when electrons in different atoms occupy positions that make the atoms form temporary dipoles (see fig. 6).

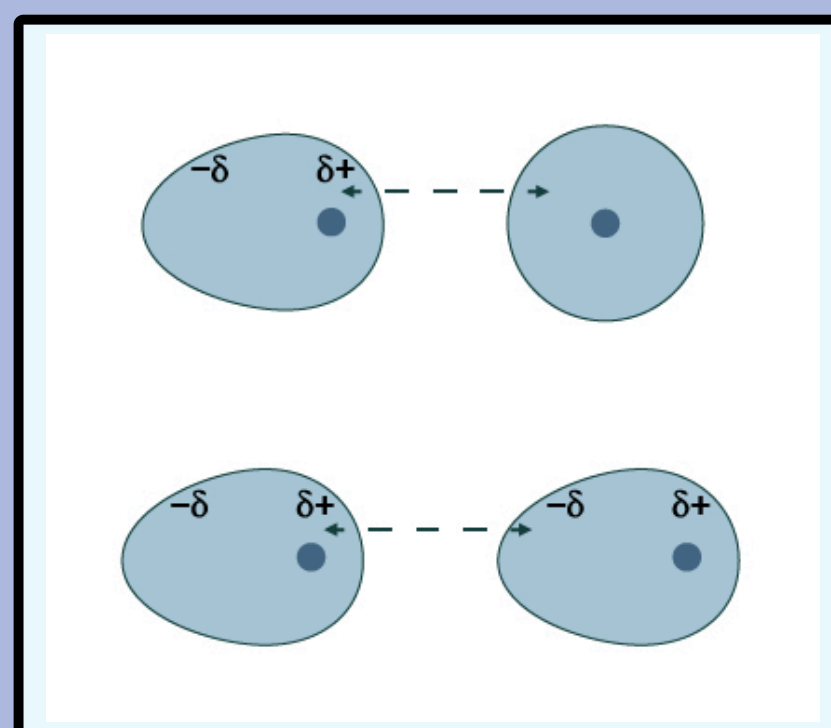


Fig. 6 LDFs

LDFs occur between all types of molecules, by chance due to the random movement of electrons. Once an uneven electron distribution momentarily occurs, it repels electrons on the same side in another atom, creating temporary partial charges and induced dipoles, as shown in fig. 6. Attractions form between these partial charges. Molecules with greater molecular weights (MW) have more atoms, which also means more electrons. This increases polarizability and leads to more frequent LDFs, because more total electrons create a higher chance that they will be on the same side.

Hydrogen Bonding

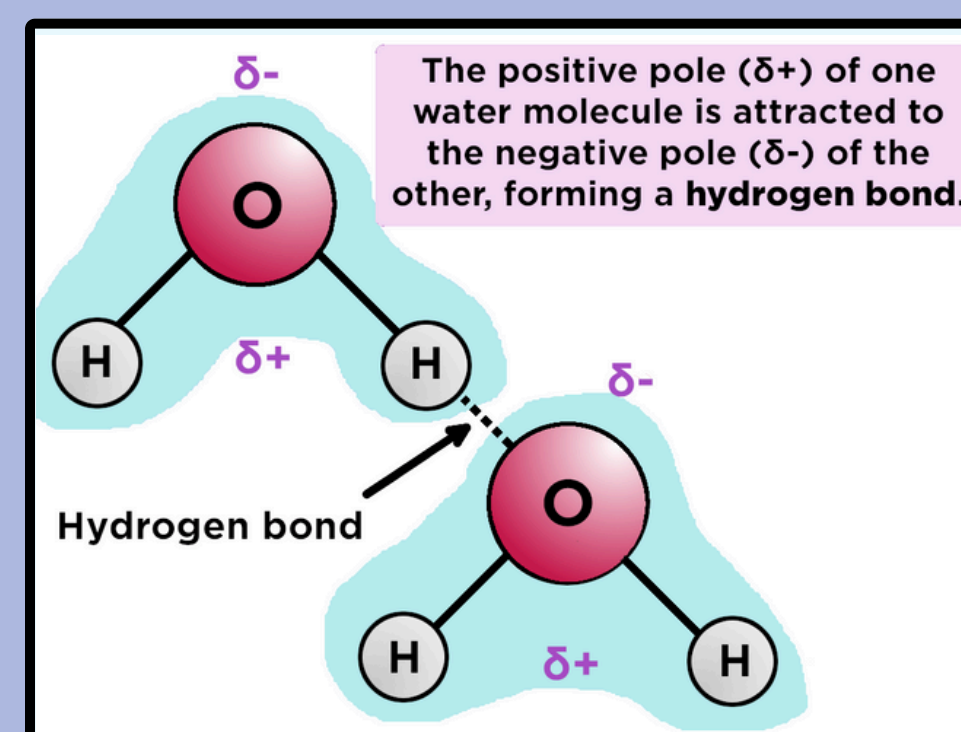


Fig. 7 Hydrogen Bonding

A hydrogen bond is a special dipole-dipole interaction between a hydrogen (bonded to N, O, or F) and another highly electronegative atom.

Fig. 7 shows that water exhibits hydrogen bonding, with the hydrogens of one atom attracted to the oxygens of another. A hydrogen bond is the strongest dipole-dipole interaction due to the low atomic radii and high partial charges of the atoms. This increases electrostatic attraction between them.

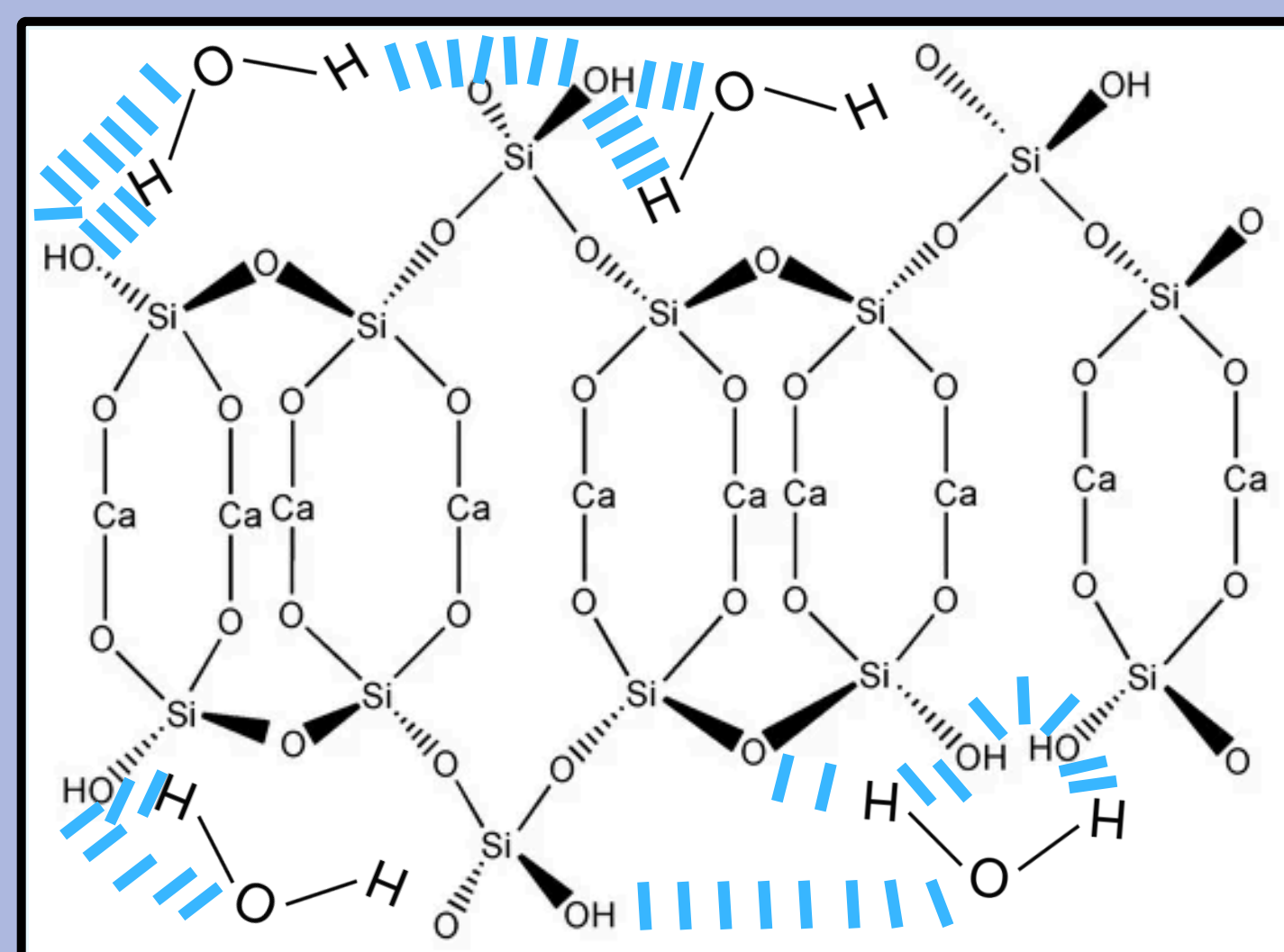


Fig. 8 IMFs Between CSH Molecules

In fig. 8, the many atoms in CaH_2SiO_4 leads to a relatively high MW, indicating more frequent LDFs. This results in a stronger attraction between CSH molecules.

Bulk Properties

For an application as the binding gel in cement

1) Initial semi-solid gel structure (to seep between all aggregate)

CSH contains two types of bonds: very polar Si-O and O-H bonds, with large electronegativity differences, and ionic $\text{Ca-H}_2\text{SiO}_4$ bonds. The polar bonds create strong bond dipoles going from Si to O and H to O. The Si-O-H group (with O as the center) has 2 bonding and 2 nonbonding domains, creating a bent structure.

In this area, the bond dipoles from H to O and Si to O do not sum to 0 since they are not opposite to each other, creating a strong molecular dipole from the O. This makes it highly polar. The large electronegativity difference in the O-H bond and the high molecular polarity of the Si-O-H group allow CSH to hydrogen bond with other CSH



molecules (consolidating and strengthening the structure). This also allows CSH to hydrogen bond with surrounding water molecules, giving it the ability to trap water. The trapped water acts as a lubricant between CSH layers, reducing rigidity and allowing it to flow somewhat freely. This creates the initial semi-solid gel structure of CSH, allowing it to get between all the aggregate in concrete. The many atoms in CSH also lead to more frequent LDFs (as stated in the previous section), contributing to increased viscosity that ensures the cement is workable and doesn't flow everywhere when poured.

2) Strengthens and hardens over time (for concrete strength)

Over time, the silica tetrahedra polymerize and form a covalent network, strengthening the structure with strong covalent bonds. The ionic bond with the Ca and the H_2SiO_4 group also strengthens and stabilizes the structure. Further, the bounded water begins to evaporate, causing it to dry out and harden.

Citations

(fig. 1, fig. 2) <https://www.youtube.com/watch?v=s1f7DzYF0jl>

(fig. 3, fig. 4, fig. 5, fig. 8) <https://www.mdpi.com/1996-1944/11/12/2367>

(fig. 6) <https://chemistry.stackexchange.com/questions/156119/why-london-dispersion-force-is-attractive-not-repulsive>

(fig. 7) <https://www.exprii.com/t/hydrogen-bonds-overview-examples-10351>

<https://www.popularmechanics.com/science/green-tech/a40785162/microalgae-carbon-neutral-cement/>