

What controls the Dissolution of Dicalcium Silicate Polymorphs?

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Dicalcium Silicate, also called belite or simply C2S in cement chemistry, accounts for ~ 30% of ordinary portland cement. It would be desirable to increase that percentage due to the possible economic and environment benefits of C2S-based cements, since C2S has a considerable lower synthesis temperature than traditional cement main component. However, C2S presents a low dissolution rate that makes it unpractical for building standards¹. Therefore, increasing the hydration rate of C2S is a long chased Holy Grail for cement industry.

It is very interesting to note that C2S dissolution is very polymorph-dependent. β -C2S, the most common form in traditional cement, has structural resemblances to the arcanite mineral family, and exhibits a much higher reaction rate with water than the γ -form, which belongs to the olivine group, and is almost inert in contact with water².

In this work in progress, we aim to understand the intrinsic difference between polymorphs that defines their disparate hydration rates, using molecular scale simulations. We are investigating the bulk crystalline structure of C2S polymorphs and the crystal-water interfacial reactions, using ab-initio and reactive force field³ molecular dynamics.

So far, we have seen that:

(i) Single water molecule adsorption/dissociation results are not enough to understand hydration, and they lead to misleading results. Hydration is a cooperative process, and it should be tackled with a more general model⁴.

(ii) Structural order can play a role in detriment to the hydration. Symmetric surfaces have very well defined water dissociation spots and distorting the surface after initial water dissociation may be tougher than for low symmetry ones².

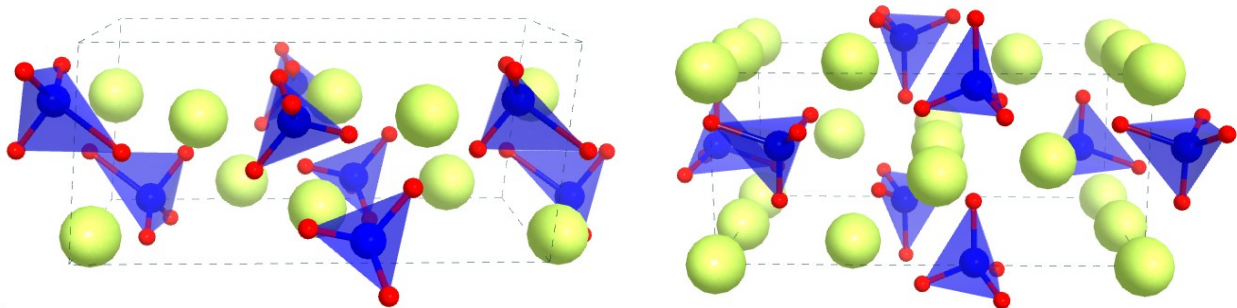


Figure 1. Representation of β -C2S (left) and γ -C2S (right) polymorphs. Ca atoms are represented in green, and silicate groups as blue tetrahedral.

Bibliography

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