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Distribution of water in synthetic calcium silicate hydrates

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Calcium silicate hydrates (C-S-H) are of main importance to understand the behavior of cement materials, as they control most of the properties [1, 2] of these man-made materials. By analogy with clay minerals, their water content and structuration at the atomic scale certain have a major influence on their properties, which needs to be assessed. Here, we used a multiple analytical approach to quantify water distribution in C-S-H samples and to determine the relative proportions of water sorbed on external and internal (interlayer) surfaces. Water vapor isotherms were used to explain the water distribution in the C-S-H microstructure. As for many layered compound, C-S-H have external and internal (interlayer) surfaces displaying multilayer adsorption of water molecules on external surfaces owing to the hydrophilic surfaces. Interlayer water was also quantified from water vapor isotherm, XRD and TGA data displaying non-reversible swelling/shrinkage behavior in response to drying/rewetting cycle. From this quantification most of the scattered data already published could be explained according to the different conditions of humidity and technics of measurement (Figure 1). Stoichiometric formula of the different C-S-H samples analyzed ($0.6 < \text{Ca/Si} < 1.6$) were proposed considering the interlayer water contribution.

Figure 1. Plots of $\text{H}_2\text{O}/\text{Si}$ against Ca/Si with the gray diamonds are adapted from 5. The blue circles are for interlayer water, the light blue ones for interlayer water and a single adsorbed monolayer and the purple ones are with the contribution of hydroxyls from this work.

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