# Structural and thermodynamic description of C-N-A-S-H

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The disordered layered hydrate phases formed in the lime-soda-alumina-silica-water (C-N-A-S-H) systems are of both technological and environmental importance, and can be formed in cementitious binders, by glass alteration, and in various other contexts. The structural resemblance between these disordered materials and the tobermorite group of minerals has long been used as a basis for their structural and thermodynamic description. However, with the incorporation of aluminium and alkalis into these phases, their composition and structure may start to differ from the standard tobermorite-derived models for C-S-H structures, particularly in terms of the cross-linking between chains which is observed at lower Ca content and in the presence of Al.

Here, we present both structural and thermodynamic models for the C-N-A-S-H phase, with a particular focus on compositions of interest in the development and analysis of alkali-activated cementitious binders. The representation of the C-N-A-S-H gel as a combination of crosslinked and non-crosslinked tobermorite structures provides significant advances in the ability to describe the chemical structures observed by $^{29}$Si MAS NMR spectroscopic analysis of these materials [1]. An 8-endmember ideal solid solution model [2] provides for the first time an accurate description of solubilities in the region of this quaternary system corresponding to the chemistry of alkali-activated cements and Portland cement blended with aluminous pozzolans. This model, when coupled with an improved description of the Mg-Al layered double hydroxide solid solution [3], is demonstrated to enable the prediction of phase assemblages and volumetric properties within alkali-activated blast furnace slag binders.

[1] Myers, Bernal, San Nicolas, Provis (2013), *Langmuir* **29**, 5294-5306. [2] Myers, Bernal, Provis (2014), *Cement and Concrete Research* **66**, 27-47. [3] Myers, Lothenbach, Bernal, Provis (2015), *Applied Geochemistry*, under review