**MS17-1-1 Structure and morphology of C-S-H-based hardening accelerator nanoparticles by X-ray total scattering techniques**
**#MS17-1-1**

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**Abstract**
Calcium silicate hydrate (C-S-H) is the main binding phase in Portland cement. The addition of C-S-H nanoparticles as nucleation seeds has successfully been used to accelerate the hydration process and the precipitation of binding phases either in conventional Portland cement or in alternative binders. Indeed, the modulation of the hydration kinetics during the early-stage dissolution-precipitation reactions, by acting on the nucleation and growth of binding phases, improves the early strength development. The fine-tuning of concrete properties in terms of compressive strength and durability by designed structural modifications can be achieved through the detailed description of the reaction products at the atomic scale. The nano-sized, chemically complex and structurally disordered nature of these phases hamper their thorough structural characterization. To this aim, we implement a novel multi-scale approach by combining forefront small-angle X-ray scattering (SAXS) and synchrotron wide-angle X-ray total scattering (WAXTS) analyses for the characterization of Cu-doped C-S-H nanoparticles dispersed in a colloidal suspension, used as hardening accelerator. SAXS and WAXTS data were analysed under a unified modelling approach by developing suitable atomistic models for C-S-H nanoparticles to be used to simulate the experimental X-ray scattering pattern through the Debye scattering equation [1]. The optimization of atomistic models against the experimental pattern, together with complementary information on the structural local order from $^{29}$Si solid-state nuclear magnetic resonance and X-ray absorption spectroscopy, provided a comprehensive description of the structure, size and morphology of C-S-H nanoparticles from the atomic to the nanometre scale. C-S-H nanoparticles were modelled as an assembly of layers composed of 7-fold coordinated Ca atoms and decorated by silicate dimers and chains. The structural layers are a few tens of nanometres in length and width, with a crystal structure resembling that of a defective tobermorite, but lacking any ordering between stacking layers [2].

**References**
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