Nanostructural and sub-nanostructural characterisation of sustainable cement

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The project aims at reconciling the macroscopic properties of sustainable cement binders with the (sub)nano-structural features of thermodynamic phases such as C-(N-)A-S-H and N-(C-)A-S-H forming by pozzolanic reaction or chemical activation in alkaline solution. These reactions can be exploited to formulate binders with reduced amounts of Portland cement, as well as Portland-free binders, leading to significant reductions in CO_2 emissions. Moreover, the partial or total replacement of Portland cement with industrial or agricultural side-stream can reduce both the amount of landfilled waste and that of extracted virgin materials.

Understanding the behaviour of these materials at the atom to nano-scale is essential for the optimisation of their engineering properties using a bottom-up approach. This goal will be addressed by combining conventional methods for mineralogical and chemical characterisation with the synthesis of phases such as C-(N-)A-S-H and N-(C-)A-S-H, having different degrees of structural disorder, and the implementation of state-of-the-art techniques for their advanced analysis. These will comprise methods based on X-ray total scattering, coupled with advanced modelling techniques relying on the Debye scattering equation (DSE) and on the pair distribution function (PDF), achieving detailed information on composition and structure at the atomic to nanometre scale. Furthermore, the implementation of methods based on neutron scattering will complement the obtained characterisation with information on nanopore topology forming by aggregation of C-(N-)A-S-H and N-(C-)A-S-H to form meso-scale clusters.

Within the scope of this project, the PhD candidate will develop advanced experimental and modelling expertise, which can be exploited in different topic areas, spanning from the characterisation of industrial minerals to the understanding of basic processes associated with the formation of mineral assemblages in diverse geological settings. The PhD candidate will also be encouraged to establish collaborations and spend period abroad with experts in the field, particularly at beamline facilities. PhD funds for research will be integrated with personal DOR funds of the supervisors as well as CIRCe funds.