



PhD project on solid-state NMR spectroscopy of cement: Aluminum in the calcium-silicate-hydrate phase

A PhD stipend is available from November 1st, 2017 or later at iNANO and the Department of Chemistry, the Faculty of Science and Technology, Aarhus University, focussing on the incorporation of aluminium in calcium-silicate-hydrate (C-S-H) phases - the principal binding component in Portland cement-based materials.

Concrete is the world's most durable, reliable and economical construction material with an annual consumption in volume by society only surpassed by water. Portland cement represents the "glue" in concrete and its world-wide production is responsible for 5 – 8 % of the man-made CO₂ emissions. The CO₂ emission originates mainly from the decarbonation of limestone (CaCO₃) and the fuels for heating the cement kilns and grinding the cement clinkers. A valuable approach to reduce CO₂ emission associated with cement production is to partly replace the Portland cement by supplementary cementitious materials such as fly ashes, slags and calcined clays. These materials are generally rich in aluminium and silicon which leads to a significant modification of the composition and structure of the C-S-H phase.

The aim of the project is to determine the structural positions of Al in C-S-H phases with different Ca/Si ratios and Al contents and to quantify the amount of Al in these different environments. These data will be implemented in thermodynamic modelling approaches which currently lack consideration of Al in the C-S-H phase. The project will mainly focus on C-S-H phases synthesized in the laboratory under different conditions. The structural and quantitative information will principally be derived from ²⁷Al and ²⁹Si solid-state NMR experiments. A part of these experiments will be conducted at the 950 MHz spectrometer at the Center for Ultrahigh Field NMR spectroscopy at iNANO. The incorporation of the results in thermodynamic modelling will be conducted in collaboration with senior scientist Barbara Lothenbach, Empa, Switzerland, and visits to Empa for at least three months are planned during the PhD study. The scientific studies will be performed in an interdisciplinary environment, utilizing the group's expertise in inorganic synthesis, structural characterization tools, solid-state NMR spectroscopy and thermodynamic modelling. A positive outcome of the project will provide new information about the C-S-H phase which will have an important impact on the design of new Portland cement blends with lower CO₂ footprint.

Qualifications and specific competences:

The PhD candidate should have a Master's (3-year PhD programme) or 4-years studies (4-year PhD programme) in chemistry, nanoscience, physics, materials science, or geology. Knowledge about inorganic materials, cement chemistry, microscale characterization tools, and NMR spectroscopy will be considered as a plus.

Application deadline and procedure:

Applications must be submitted electronically, following the procedure described on the following site:

<http://talent.au.dk/phd/scienceandtechnology/opencalls/calls-on-specific-projects/august-2017/solid-state-nmr-spectroscopy-of-cement-aluminum-in-the-calcium-silicate-hydrate-phase/>

The deadline for applications is **August 1st, 2017**.

Applicants seeking further information are invited to contact: Assoc. Prof. Jørgen Skibsted, Department of Chemistry and iNANO, Langelandsgade 140, DK-8000C Aarhus, Denmark, e-mail: jskib@chem.au.dk, phone +45 2899 2029.