Abstract
With the world facing a climate crisis due to increasing CO$_2$ emissions, there is pressing need to develop and implement sustainable construction/engineering materials across the globe. Alkali-activated materials (AAMs) are one such sustainable alternative to conventional Portland cement concrete; yet questions remain regarding the long-term behavior of AAMs. Furthermore, for Portland cement, the use of extensive clinker substitution to reduce CO$_2$ emissions has led to changes to the underlying chemistry of the main binder gel (calcium-silicate-hydrate, C-S-H, gel), where it is uncertain how these novel supplementary cementitious materials augment the long-term behavior (e.g., gel stability and pore structure) of the cement binder. In this talk, I will outline how fundamental materials science research is being used to address the long-term behavior unknowns of AAMs and certain Portland cement-based systems, where we are linking key experimental techniques with atomistic and larger length scale simulations. In particular, to assess gel stability in calcium-rich AAMs, we have used density functional theory (DFT), synchrotron-based X-ray pair distribution function (PDF) analysis and nuclear magnetic resonance (NMR) to investigate the influence of alkali and alumina incorporation on the structure and thermodynamics of C-S-H gel. The DFT results point toward a clear upper limit for sodium incorporation, beyond which the stability of the phase is compromised, while the experimental results show how alumina can be utilized to combat the destabilizing effects of sodium. We have also used DFT to uncover the early-stage formation behavior of C-S-H gel and the influence of sodium and alumina, which has led to a tentatively proposed formation mechanism of the gel.

Dr. Claire White
Associate Professor, Princeton University

Claire White is an associate professor in the Department of Civil and Environmental Engineering and the Andlinger Center for Energy and the Environment, and is the acting associate director for research in the Andlinger Center for Energy and the Environment. She holds associated faculty status in the Departments of Chemical and Biological Engineering, and Mechanical and Aerospace Engineering, the Princeton Institute for the Science and Technology of Materials, High Meadows Environmental Institute, and Princeton Institute for Computational Science and Engineering. She completed her graduate studies in 2010 at the University of Melbourne supported by an Australian Postgraduate Award from the Australian government. After receiving her PhD, she worked as a postdoc at Los Alamos National Laboratory and was awarded a Director’s Postdoctoral Fellowship to research the atomic structure of low-CO$_2$ alkali-activated materials. In 2013 she joined Princeton University. Professor White is the recipient of a number of awards including an NSF CAREER Award, the RILEM Gustavo Colonnetti Medal, and the Howard B. Wentz Jr. Junior Faculty Award (Princeton University) and has been listed numerous times on the Princeton Engineering Commendation List for Outstanding Teaching.

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