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Gelation of calcium-silicate-hydrate in cement KATERINA IOANNIDOU, MSE2, joint MIT-CNRS lab, MIT, Cambridge, MA 02139, US, MATEJ KANDUC, Department of Physics, Free University Berlin, D-14195 Berlin, Germany, LUNNA LI, DAAN FRENKEL, Department of Chemistry, University of Cambridge, Cambridge, UK, JURE DOBNIKAR, IRCSM, Beijing University of Chemical Technology, Beijing, P. R. China, ROLAND PELLENQ, MSE2, joint MIT-CNRS lab, MIT, Cambridge, MA 02139, US, EMANUELA DEL GADO, Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University, Washington, DC 20057, US — The calcium-silicate-hydrate (C-S-H) gel forms and densifies via precipitation and aggregation of nano-scale hydrates within a couple of hours during cement hydration and it is the main responsible for cement strength. We have investigated equilibrium and arrested states representative of the effective interactions between the nano-scale C-S-H at different stages of the hydration. The inter-hydrate interactions are due to ion correlation forces arising from strong surface charge heterogeneities and change from repulsive to strongly attractive during the early stages of cement hydration, according to the ionic concentration. We analyze the cluster size distributions, the morphology, the local packing and the free energy of aggregates and crystalline phases, using molecular dynamics and Monte Carlo simulations. We compare the results of equilibrium calculations with non-equilibrium simulations that capture the main features of the hydration kinetics. The emerging picture is that the evolving effective interactions provide a thermodynamic driving for the growth of the gel and for its continuous densification that is crucial to cement strength.

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