

UNIVERSITY of HOUSTON

CULLEN COLLEGE of ENGINEERING

Department of Civil & Environmental Engineering

CIVE 6111 Graduate Seminar Series

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Civil and Environmental Engineering
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Structure and Properties of Calcium Silicate Hydrates

Friday, November 4, 2016

2:45 pm – 3:45pm

Classroom Business Building, 120

Abstract: In American infrastructure report card, ASCE gives an unsatisfactory D+ grade to the U.S. infrastructure. This report reaffirms the long known dire condition of our degrading civil infrastructure that calls for immediate financial investment, basic research and public education. To date, the fundamental mechanisms behind the long-term performance of concrete and cementitious materials remain to be obscure. In this talk, we focus on calcium silicate hydrates (C-S-H), the major binding phase in concrete that is responsible for its strength and durability. We first present our recent efforts in developing consistent molecular models of C-S-H. In light of these new models, we explore chemophysical origins of C-S-H's thermo-mechanical properties at the nano- and meso-scale. To this end, we first investigate whether nano-mechanical properties of C-S-H are driven by defects or density. Second, we examine the possibility of decreasing the thermal conductivity of C-S-H without reducing its mechanical properties. Finally, we discuss the role of intermolecular forces between C-S-H nano-layers in determining C-S-H's mechanical properties and the prospect of creating chemistry-dependent meso-scale structures of C-S-H.

About the speaker:



Mohammad Javad Abdolhosseini Qomi, Ph.D. is an assistant professor in the department of civil and environmental engineering, at the University of California, Irvine. He has 10+ years' worth of experience developing and employing atomistic simulation to study the mechano-physical properties of materials at the nanoscale. Besides his home-built software packages, he has and continues to contribute to the development of open source molecular dynamics software packages such as GULP (Curtin University, AUS) and LAMMPS (Sandia National Lab, USA). For the past 7 years, he has employed atomistic simulation techniques to study the impact of chemical composition on the mechanical and physical properties of cementitious materials at the nanoscale. This includes investigation of chemical composition such as calcium-to-silicon ratio on the structure, elasticity, strength and fracture toughness of calciumsilicates phases in hardened cement paste. His current research aims to discover the underlying physical chemistry processes controlling durability of cementitious materials in extreme conditions pertinent to the oil well cementing, nuclear waste disposal and carbon sequestration. To this end, he uses multi-scale and multi-physics modeling of the degradation and aging phenomenon in cementitious materials with particular emphasis at the nano- and meso-scales. His research on cementitious materials are featured in various journals including, Nature Communications, Physical Review Letters, Journal of Physical Chemistry, Chemical Physics, American Ceramics Society, to name a few. He is an active member of the Engineering Mechanics Institute and American Ceramics Society Cement Division.