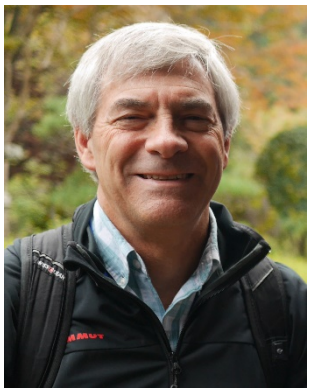
The Department of Civil and Environmental Engineering at the University of Houston presents...

CIVE 6111 Graduate Seminar

An *in situ* look at the relationship between interfacial solution structure, mineral nucleation and colloidal assembly



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Friday, November 22, 2019
2:45pm-3:45pm
Classroom Business Building (CBB) – Room 118

Abstract
Heterogenseous distributions of ions and water at mineral interfaces leads to a range of phenomena with widespread consequences for natural and synthetic processes, including sequestration of solution species, heterogeneous nucleation, and growth of nanostructured materials via colloidal assembly. Using a combination of *in situ* imaging techniques and computational methods, we are investigating these phenomena and their relationship to interfacial strcuture for a number of systems including phyllosilicates, aluminum hydroxides, and iron and zinc oxides. For example, using high speed, atomically resolved AFM to directly observe gibbsite formation from $AlCl_3$ solutions on muscovite mica, we quantify the ion adsorption, dynamics of sub-critical clusters and the transition to stable gibbsite films. We compare these results to the predictions of classical nucleation theory and use DFT simulations and triple layer models to relate the behavior to the underlying ion distributions and surface interactions. In the iron oxide system, we combine high temperature *in situ* TEM with classical DFT simulations to investigate the impact of organics on the transformation of ferrihydrite to hematite (Hm). We show that addition of oxalate induces interfacial gradients in ion concentration that cause nucleation to be restricted to an interfacial region about 1 nm away from any existing hematite particle, to which they then immediately attach. This process is repeated at a regular orientation-specific rates, leading to the formation of complex mesocrystals that are self-similar at all times. Finally, we show how we can directly image solution structure with sub-nm lateral and vertical resolution using AFM-based fast force mapping applied to mica- and boehmite-water interfaces. We separate the measured force gradients into long range dispersion interactions and short range solvation forces and compare the results to predictions from MD simulations to reveal how water is distributed amongst the various atomic sites on the surface. Taken together, these results begin to build a coherent picture of mineral-water interfacial structure and its control on ion adsorption, interface-driven nucleation and interpartcle forces.

Bio
Jim De Yoreo is a Battelle Fellow and Chief Scientist for Materials Science in the Physical and Computational Sciences Directorate at Pacific Northwest National Laboratory (PNNL), an Affiliate Professor of Materials Science and Engineering and of Chemistry at the University of Washington, and Co-Director of the Northwest Institute for Materials Physics, Chemistry and Technology (NW IMPACT). He received his PhD in Physics from Cornell University in 1985. Following post-doctoral work at the University of Maine and at Princeton University, he became a member of the technical staff at Lawrence Livermore National Laboratory in 1989, where he held numerous positions. He joined Lawrence Berkeley National Laboratory in 2007 where he served as Deputy and then Interim Director of the Molecular Foundry before moving to PNNL in 2012. De Yoreo's research has spanned a range of materials-related disciplines, focusing recently on interactions, assembly, and crystallization in inorganic, biomolecular and biomineral systems. De Yoreo has authored, co-authored, or edited over 250 publications and patents. He is a recipient of the David Turnbull Lectureship of the Materials Research Society (MRS), the Laudise Prize of the International Organization for Crystal Growth (IOCG) and the Crystal Growth Award of the American Association for Crystal Growth (AACG). He served as President of the MRS and he is a Fellow of the American Physical Society and the MRS, and a member of the Washington State Academy of Sciences and the IOCG and AACG Executive Committees.