Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Nanoscale Charge Balancing Mechanism in Calcium-Silicate-Hydrate Gels: Novel Complex Disordered Materials from First-principles[1] ONGUN OZCELIK, CLAIRE WHITE, Princeton Univ — Alkali-activated materials which have augmented chemical compositions as compared to ordinary Portland cement are sustainable technologies that have the potential to lower CO_2 emissions associated with the construction industry. In particular, calcium-silicate-hydrate (C-S-H) gel is altered at the atomic scale due to changes in its chemical composition. Here, based on first-principles calculations, we predict a charge balancing mechanism[1] at the molecular level in C-S-H gels when alkali atoms are introduced into their structure. This charge balancing process is responsible for the formation of novel structures which possess superior mechanical properties compared to their charge unbalanced counterparts. Different structural representations are obtained depending on the level of substitution and the degree of charge balancing incorporated in the structures. The impact of these charge balancing effects on the structures is assessed by analyzing their formation energies, local bonding environments, diffusion barriers and mechanical properties. These results provide information on the phase stability of alkali/aluminum containing C-S-H gels, shedding light on the fundamental mechanisms that play a crucial role in these complex disordered materials. [1] arXiv:1610.00112

[1]We acknowledge funding from the Princeton Center for Complex Materials, a MRSEC supported by NSF.

Ongun Ozcelik
Princeton Univ

Date submitted: 11 Nov 2016 Electronic form version 1.4