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Education

Joint PhD in Civil and Environmental Engineering and Materials Science	2016 – 2020
Princeton University (PU), USA	
Thesis: "Gel and Pore Structure Formation in Alkali-activated Materials"	
Graduate Certificate in Computational and Information Science	
MS in Civil and Environmental Engineering	2014 - 2016
Princeton University (PU), USA	
BEng (First Class Honor) in Civil Engineering	2011 – 2014
The University of Hong Kong (HKU), China	

Publications

- (1) Gong, K.; **Yang, K.**; White, C. E. Density Functional Modeling of the Binding Energies between Aluminosilicate Oligomers and Different Metal Cations. *Front. Mater.* 2023, 10.
- (2) **Yang, K.**; White, C. E. Modeling of Aqueous Species Interaction Energies Prior to Nucleation in Cement-Based Gel Systems. *Cem. Concr. Res.* 2021, 139, 106266.
- (3) Gong, K.; Özçelik, V. O.; **Yang, K.**; White, C. E. Density Functional Modeling and Total Scattering Analysis of the Atomic Structure of a Quaternary CaO-MgO-Al₂O₃-SiO₂ (CMAS) Glass: Uncovering the Local Environment of Magnesium. *Phys. Rev. Mater.* 2021, 5 (1), 015603.
- (4) **Yang, K.**; White, C. E. Multiscale Pore Structure Determination of Cement Paste via Simulation and Experiment: The Case of Alkali-Activated Metakaolin. *Cem. Concr. Res.* 2020, 137, 106212.
- (5) Salganik, M. J.; Lundberg, I.; Kindel, A. T.; Ahearn, C. E.; Al-Ghoneim, K.; Almaatouq, A.; Altschul, D. M.; Brand, J. E.; Carnegie, N. B.; Compton, R. J.; et al. Measuring the Predictability of Life Outcomes with a Scientific Mass Collaboration. *Proc. Natl. Acad. Sci.* 2020, 117 (15), 8398 LP – 8403.
- (6) **Yang, K.**; Özçelik, V. O.; Garg, N.; Gong, K.; White, C. E. Drying-Induced Atomic Structural Rearrangements in Sodium-Based Calcium-Alumino-Silicate-Hydrate Gel and the Mitigating Effects of ZrO₂ Nanoparticles. *Phys. Chem. Chem. Phys.* 2018, 20 (13), 8593–8606. (**part of 2018 PCCP HOT Articles**)
- (7) Gu, T.; Jeong, H.; **Yang, K.**; Wu, F.; Yao, N.; Priestley, R. D.; White, C. E.; Arnold, C. B. Anisotropic Crystallization in Solution Processed Chalcogenide Thin Film by Linearly Polarized Laser. *Appl. Phys. Lett.* 2017, 110 (4), 41904.

- (8) **Yang, K.;** White, C. E. Modeling the Formation of Alkali Aluminosilicate Gels at the Mesoscale Using Coarse-Grained Monte Carlo. *Langmuir* 2016, 32 (44), 11580–11590.

Conference Presentations

Yang K, White CE, Multiscale pore structure determination of alkali-activated metakaolin via simulation and experiment: Micropores to macropores, 10th Advances in Cement Based Materials, University of Illinois at Urbana-Champaign, Urbana, USA, 16-18 June 2019 (Oral)

Yang K, White CE, Density functional modeling of the pre-nucleation clusters of calciumsilicate-hydrate and related gels, 9th Advances in Cement-Based Materials, University Park, Pennsylvania, USA, 11-12 June 2018 (Oral)

Yang K and White CE, *Modeling the formation of sodium and calcium aluminosilicate gels at the mesoscale using coarse-grained Monte Carlo*, Gordon Research Conference on Neutron Scattering, August 6 – 11, 2017, Hong Kong, China (Poster)

Yang K and White CE, *Modeling the formation of sodium and calcium aluminosilicate gels at the mesoscale using coarse-grained Monte Carlo*, 253rd ACS National Meeting, April 2-6, 2017, San Francisco, California, USA (Oral)

Yang K and White CE, *Does gel stability play a role in dictating the extent of microcracking in alkali-activated slag paste?*, 6th International Conference on Engineering for Waste and Biomass Valorisation, May 23 – 26, 2016, Albi, France (Oral flash + poster)

Yang K and White CE, *A mesoscale investigation of the alkali-activation reaction using coarse-grained Monte Carlo simulations*, 6th Advances in Cement-based Materials, July 20 – 22, 2015, Manhattan, Kansas, USA (Oral)

Other Presentations

Yang K, Özçelik VO, Garg N, Gong K and White CE, *Drying-Induced Atomic Structural Rearrangements in Sodium-Based Calcium-Alumino-Silicate-Hydrate Gel and the Mitigating Effects of ZrO₂ Nanoparticles*, PRISM Annual Research Symposium, March 13 – 14, 2018, Princeton, New Jersey, USA (Poster)

Yang K and White CE, *Density functional modeling of interactions between hydrated calcium clusters and aluminosilicate species*, Princeton E-Filiates Partnership 2017 Annual Meeting, November 10, 2017, Princeton, New Jersey, USA (Poster)

Yang K and White CE, *Does gel stability play a role in dictating the extent of microcracking in alkali-activated slag paste?*, Princeton E-filiates Partnership 2016 Retreat, January 28 – 29, 2016, Princeton, New Jersey, USA (Poster)

Yang K and White CE, *A mesoscale investigation of the alkali-activation reaction using coarse-grained Monte Carlo simulations*, Princeton E-Filiates Partnership 2015 Annual Meeting, November 20, 2015, Princeton, New Jersey, USA (Poster)

Teaching Experience

Assistant in Instruction

- ENE 267: *Materials for Energy Technologies and Efficiency*, Fall 2018
- CEE 364: *Materials in Civil Engineering*, Spring 2014, 2015
- CEE 102: *Engineering in the Modern World*, Fall 2014, 2015
- CEE 262: *Structures and the Urban Environment*, Spring 2014

Honors & Awards

Nanocem PhD Award Finalist	2020
Graduate Student Fellowship, PU	2016
WasteEng2016 Conference Best Student Poster Award	2016
University Research Fellowship Program, HKU	2013
Hong Kong University Worldwide Scholarship	2012
Dean's Honors List, HKU	2012