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Comptational Design Of Functional CA-S-H and Oxide Doped Alloy Systems[1] SHIZHONG YANG, LOKESHWAR CHILLA, YAN YANG, KUO LI, SCOTT WICKER, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, SHUJU BAI, Southern University and AM College, BOLIANG ZHANG, SHENGMIN GUO, Louisiana State University — Computer aided functional materials design accelerates the discovery of novel materials. This presentation will cover our recent research advance on the Ca-S-H system properties prediction and oxide doped high entropy alloy property simulation and experiment validation. Several recent developed computational materials design methods were utilized to the two systems physical and chemical properties prediction. A comparison of simulation results to the corresponding experiment data will be introduced.

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