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Nanoscale Properties and Stability Simulations of Alkali Activated Cement Phases from First Principle Calculations ONGUN OZCELIK, CLAIRE WHITE, Princeton University — Using first principle density functional calculations, we present the nanoscale properties of interactions, local bonds, charge distributions, mechanical properties and strength of alkali activated cement phases which are the most promising alternative to the ordinary Portland cement with a much lower cost to the environment. We present results on the stability and long term durability of various alkali activated cement structures, effects of external alkali agents on their properties and ways of utilizing them for further applications. We compare the calculated properties of alkali activated cement with those of ordinary Portland cement and contribute to the formation of long term durability data of these phases. Comparison with X-ray and neutron scattering experiment results are also provided via pair distribution functions extracted from simulation results.

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