Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Microscopic Understanding of Reactivity of Clinkers for Green Cement ENGIN DURGUN, HEGOI MANZANO, ROLAND J. M. PELLENQ, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Cement is the cause of up to 10 percent of global CO2 emissions, and yet, while it is one of the most common materials in use, we have remarkably little understanding of its microscopic properties. Toward this end, we use quantum mechanical simulations to examine the electronic properties and structure of cement crystals and to understand the surface reactivity of various clinker phases. Using these results, our aim is to clarify the mechanisms of cement dissolution, which is the initial stage of hydration and also one of the key processes that leads to the need for high temperature/energy manufacturing. As a first step we modeled the crystal structure of two major clinker phases, alite and belite and analyzed both electronic and mechanical properties. Next, we cleaved the clinker crystal in the simulation along different symmetry directions in order to obtain a prediction of the most stable surfaces. Dissolution occurs at the surface so accurate determination of the surface pattern is crucial. Using the computed surface energies, we can predict the full structure of the clinker nanocluster. This allows us to examine the interaction of water molecules with different nanocluster phases, in order to shed light on the dissolution mechanism and use this new understanding to predict possible novel routes for modifying and controlling the dissolution reactions.

Engin Durgun
Massachusetts Institute of Technology

Date submitted: 19 Nov 2010 Electronic form version 1.4