Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Surface reactivity/stability and hydration of calcium silicate phases ENGIN DURGUN, Massachusetts Institute of Tecnology and UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, CAN ATACA, HAMLIN M. JENNINGS, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Recent studies on synthetic calcium silicate structures revealed important mechanisms to tune the reactivity of various cement phases. Interaction of water with dicalcium silicate (C2S-belite) and tricalcium silicate (C3S-alite), dominant phases in Portland Cement, are the most important and anticipated reactions. In this work, using first-principles calculations, a fundamental understanding of how water pressure affects the reactivity of C3S and C2S phases is provided. In order to understand the hydration of different phases, as a first step the surface energetics of all lower index orientations are calculated and the stability/reactivity of the surfaces are determined. Taking into account the most and least energetic surfaces of the C3S phase, detailed analyses are carried out in order to understand the induction period in hydration. Surface transformation from highly reactive C3S to low reactive C2S revealed that upon increasing the water pressure, the surface with C2S character becomes energetically more favorable. Reduction of the surface energy is more intense in the case of proton exchange of surface Ca atoms. Our calculations suggest that these processes are the most probable mechanisms underlying the rapid decrease in reactivity in alite hydration.

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Date submitted: 27 Nov 2012 Electronic form version 1.4