Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Modeling the Local Structure of Amorphous Materials: A Density Functional Theory Investigation**[1] KAI GONG, ONGUN OZCELIK, CLAIRE WHITE, Princeton Univ — Here, we present an iterative methodology alternating between density functional theory (DFT) calculations and pair distribution function (PDF) analysis to uncover the detailed atomic structure of highly amorphous materials. In this methodology, the DFT calculations are used to maintain chemical feasibility of the atomic structure, while the experimentally-driven refinements allow for exploration of the potential energy landscape. Through this iterative process, a final structure is obtained that is not only thermodynamically favorable but also in agreement with experiment data. Previously, we have demonstrated the applicability of similar DFT-PDF iterative methods in metakaolin and amorphous magnesium carbonate. Here, we have modified the methodology and applied it to resolve the atomic structure of ground granulated blast-furnace slag, a highly disordered calcium-magnesium aluminosilicate glassy material. Prior to applying the iterative process, a high temperature molecular dynamics (MD) simulation was used to generate a reasonable starting structure, which was found to be crucial. The iterative methodology outlined here is expected to be readily transferable to other disordered material systems where detailed atomic structures are currently not available.

[1]This material is based on work supported by the National Science Foundation under Grant No. 1362039

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Date submitted: 11 Nov 2016 Electronic form version 1.4