

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Large DFT: to 100K atoms and beyond.** JONATHAN MULLIN, Army Research Laboratory — A quantum mechanical (QM) approach to materials science provides a gold standard atomistic picture of the mechanisms responsible for a range of phenomena seen in macroscopic and experimental situations. The need to understand materials science problems from atomistic to macroscale was the impetus for ARL to initiate the Enterprise for Multiscale Material Research. This long term project attempts to redefine how materials science questions are posed, and solved. To support this goal, current state-of-the-art QM capabilities need to be extended in the number of atoms which can be treated and the length scale of the dynamics which can be simulated. This extension is referred to as large scale QM, both large spatially and temporally. This will enable fundamental advances in the understanding of materials science problems.

Jonathan Mullin  
Army Research Laboratory

Date submitted: 06 Nov 2015

Electronic form version 1.4