Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Evolutionary optimization of PAW data-sets for accurate high pressure simulations[1] KANCHAN SARKAR, Univ of Minnesota - Twin Cities , MEHMET TOPSAKAL, Brookhaven National Lab, NATALIE HOLZWARTH, Wake Forest University, RENATA WENTZCOVITCH, Univ of Minnesota - Twin Cities — We examine the challenge of performing accurate electronic structure calculations at high pressures by comparing the results of all-electron full potential linearized augmented-plane-wave calculations with those of the projector augmented wave (PAW) method. In particular, we focus on developing an automated and consistent way of generating transferable PAW data-sets that can closely produce the all electron equation of state defined from zero to arbitrary high pressures. The technique we propose is an evolutionary search procedure that exploits the ATOMPAW code to generate atomic data-sets and the Quantum ESPRESSO software suite for total energy calculations. We demonstrate different aspects of its workability by optimizing PAW basis functions of some elements relatively abundant in planetary interiors. In addition, we introduce a new measure of atomic data-set goodness by considering their performance uniformity over an enlarged pressure range.

[1]This work is supported primarily by grants NSF/EAR 1348066 and NSF/DMR 1503084. Computations are performed at the Minnesota Supercomputing Institute (MSI).

Kanchan Sarkar
Univ of Minnesota - Twin Cities

Date submitted: 10 Nov 2016 Electronic form version 1.4