

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Efficient mixing scheme for self-consistent all-electron charge density** TATSUYA SHISHIDOU, Hiroshima University, MICHAEL WEINERT, University of Wisconsin, Milwaukee — In standard *ab initio* density-functional theory calculations, the charge density  $\rho$  is gradually updated using the “input” and “output” densities of the current and previous iteration steps. To accelerate the convergence, Pulay mixing has been widely used with great success. It expresses an “optimal” input density  $\rho^{\text{opt}}$  and its “residual”  $R^{\text{opt}}$  by a linear combination of the densities of the iteration sequences. In large-scale metallic systems, however, the long range nature of Coulomb interaction often causes the “charge sloshing” phenomenon and significantly impacts the convergence. Two treatments, represented in reciprocal space, are known to suppress the sloshing: (i) the inverse Kerker metric for Pulay optimization and (ii) Kerker-type preconditioning in mixing  $R^{\text{opt}}$ . In all-electron methods, where the charge density does not have a converging Fourier representation, treatments equivalent or similar to (i) and (ii) have not been described so far. In this work, we show that, by going through the calculation of Hartree potential, one can accomplish the procedures (i) and (ii) without entering the reciprocal space. Test calculations are done with a FLAPW method.

Tatsuya Shishidou  
Hiroshima University

Date submitted: 13 Nov 2014

Electronic form version 1.4