

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**The optimized effective potential of meta-generalized gradient approximations in solids**<sup>1</sup> ZENGHUI YANG, JOHN PERDEW, Department of Physics, Temple University — Unlike the local density approximation(LDA) and the generalized gradient approximation(GGA), calculations with meta-GGAs are usually done according to the generalized Kohn-Sham(gKS) formalism. The exchange-correlation potential of the gKS equation is non-multiplicative, which prevents systematic comparison of meta-GGA bandstructures to those of the LDA and the GGA. We implement the optimized effective potential(OEP) of the meta-GGA for periodic systems, which allows us to carry out meta-GGA calculations in the same KS manner as for the LDA and the GGA. We apply the OEP to several popular meta-GGAs, including the new SCAN functional[Phys. Rev. Lett. 115, 036402(2015)]. We find that the KS gaps of meta-GGAs are close to those of GGAs, and they are smaller than the gKS gaps of meta-GGAs. The well-known grid sensitivity of meta-GGAs is much more severe in OEP calculations.

<sup>1</sup>The authors are supported by the National Science Foundation(Grant No. DMR-1305135).

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Date submitted: 06 Nov 2015

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