

Abstract Submitted  
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**A More Accurate Generalized Gradient Approximation for Solids**<sup>1</sup> ZHIGANG WU, RONALD E. COHEN, Carnegie Institution of Washington — We present a new nonempirical density functional generalized gradient approximation (GGA) based on a diffuse radial cutoff for the exchange-hole in real space and the analytic gradient expansion of the exchange energy for small gradients. There are no adjustable parameters, the constraining conditions of PBE are maintained, and the functional is easily implemented in existing codes. For the 18 testing solids including simple and transition metals, and ionic and covalent crystals, the new functional improves equilibrium lattice constants and bulk moduli significantly over the most popular Perdew-Burke-Ernzerhof (PBE) GGA and the local density approximation (LDA), and its accuracy for cohesive energies is similar to PBE. It also predicts highly accurate ground states of ferroelectrics, better metal surface energies and sublimation energy of ice than PBE and LDA, and correct ground states of magnetic iron and alpha quartz.

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