

Empirical Laplacian-based model of the adiabatic exchange-correlation energy density in Si

Antonio C. Cancio

*Department of Physics and Astronomy, Ball State University
Muncie, IN 47304*

M. Y. Chou

*Department of Physics, Georgia Institute of Technology
Atlanta GA, 30332*

We explore density functional theory (DFT) models based on the Laplacian of the local density, and derived from a fit to accurate variational Monte Carlo (VMC) data for the adiabatic exchange-correlation energy density of the Si crystal. Corrections to the exchange-correlation potential generated by Laplacian terms have been implemented within a pseudopotential plane-wave scheme and the effects on electronic structure of the crystal has been explored. We find that the rms discrepancy between the local density approximation and the VMC data is reduced 70% using a three-parameter correction to the LDA that incorporates the local Laplacian only, with similar reductions in error found for the Si atom with no modification to the model. Self-consistent calculations of structural properties of Si reproduce those of the LDA. In contrast, the local gradient of the density provides an insignificant improvement to the fit, while its incorporation results large and unphysical features into the exchange-correlation potential, and significantly poorer description of structural properties.