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Empirical Laplacian-based model of the exchange-correlation energy density and potential in Si A.C. CANCIO, Ball State University, M.Y. CHOU, Georgia Tech — We explore density functional theory (DFT) models based on the Laplacian of the local density, derived from a fit to accurate variational Monte Carlo (VMC) data for the adiabatic exchange-correlation energy density of the Si crystal. We find that the rms discrepancy between the local density approximation (LDA) and the VMC data is reduced 70% using a three-parameter correction to the LDA that incorporates the local Laplacian only, with a similar reduction in error for the Si atom with no modification to the model. Corrections to the LDA exchange-correlation potential generated by Laplacian terms have been implemented within a pseudopotential plane-wave scheme. Self-consistent calculations of the structural properties of Si using this potential reproduce those of the LDA. In contrast, the local gradient of the density provides an insignificant improvement to the fit, while introducing unphysical features into the exchange-correlation potential, and giving a significantly poorer description of structural properties. Application of our model to other semiconductors will be briefly discussed.

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