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Exchange energy and potential using the Laplacian of the density

CHRIS WAGNER, ANTONIO CANCIO, Ball State University — abstract- The challenge of density functional theory is the useful approximation of the exchange correlation energy. This energy can be approximated with the local electron density and the gradient of the density. Many different GGA's have been made recently and there is controversy over the best overall functional. Recent Monte Carlo simulations give evidence that the Laplacian of the density might be a better starting place than the gradient to correct the local density approximation. It also gives a better representation of the exchange potential at the nuclear cusp and of bonding between atoms. We have tested several Laplacian based GGA models for exchange for small atoms. We use known constraints on the exchange energy used in current GGA's. In many models unphysical oscillations occur in the potential, and understanding and eliminating them is part of the focus of this research. Preliminary results suggest that smaller values for short and long range constraints in the literature give more physically reasonable results in the Laplacian models.

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