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Real-Space DFT Models for Strong Correlation

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Accurate treatment of strongly-correlated electrons remains an important challenge for density-functional theory. Most functionals underestimate the energy lowering arising from non-dynamical electron correlation, as in stretched covalent bonds, open-shell singlet states, and many transition-metal compounds, including semiconductors. We develop a new density-functional approach combining physical insight from chemical structure with real-space modeling of the exchange-correlation hole, based on the Becke-Roussel exchange functional. The method is capable of predicting correct dissociation limits and describing strong correlation in many-electron systems.