

Abstract Submitted
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Quest for a workhorse MGGA functional BERNARD DELLEY, Paul Scherrer Institut — A semi-empirical, numerically robust, parametrization of the exchange functional has been obtained by optimization of bond energies in a database of 500 species. The variables, density, gradient and kinetic energy density, can differentiate efficiently among the wide variety of bonds in the database. The resulting MGGA rivals the thermochemistry accuracy of composite quantum chemistry approaches when applied to a wider data set. But, not only, it also provides noticeable improvements over GGA's for solid state properties, including properties not obviously related to bonding energies. As an MGGA is not significantly more demanding computationally than a GGA, this MGGA may become the workhorse density functional for a wide range of applications.

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