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Quest for a semi-empirical MGGA functional with tight bound

BERNARD DELLEY, Paul Scherrer Inst — A numerically robust parametrization for a meta-GGA exchange functional approximation has been obtained by optimization of bond energies in a database of 303 species.The variables, density, gradient and kinetic energy density, are useful to differentiate efficiently among the wide variety of bonding types in the database. The resulting MGGA rivals the thermochmistry accuracy of composite quantum chemistry approaches when applied to a wider data set of 592 species. Noticeable improvements over GGA's are also obtained for solid state properties. The present functional shows some similarities with the recently presented SCAN functional of Sun, Ruscinszky and Perdew. With the easily available semi-nonlocality through gradients and a kinetic energy density,this MGGA is widely widely applicable for molecular- as well as for extended systems and surface models.

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