Abstract Submitted
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Self-Interaction Free and Analytic Treatment of the Coulomb Energy in Kohn-Sham Density Functional Theory[1] MARKUS DAENE, ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We have developed a new treatment of the LDA functional in Kohn-Sham density functional theory which is expressed in terms of the pair density of a non-interacting system of particles, thus avoiding from the outset self-interaction effects. The pair density is expressed explicitly in terms of the density using a orthonormal and complete basis expressed as a functional of the density. This allows its functional differentiation with respect to the density and therefore the determination of the self-interaction free Coulomb potential by analytic means. The method is illustrated with numerical results for the atom series.

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