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Self-interaction-free nonlocal correlation energy functional associated with a Jastrow function[1] NAOTO UMEZAWA, National Institute for Materials Science, BRIAN AUSTIN, WILLIAM A. LESTER, JR, University of California, Berkeley and Lawrence Berkeley National Laboratory — We propose a self-interaction-free nonlocal correlation energy functional based on the transcorrelated method [1]. An effective Hamiltonian, $\mathcal{H}_{\text{eff}} = \frac{1}{F}\mathcal{H}F$, is derived from a similarity transformation with respect to a 'Jastrow' correlation factor, F. The total energy is given by the expectation value of $\mathcal{H}_{\text{eff}}$ with respect to a single Slater determinant. If a two-body Jastrow function is adopted, the resulting method resembles a Kohn-Sham density functional theory in which the correlation energy functional consists of two- and three-body interactions [2]. To simplify our calculations, we exclude the three-body terms and instead multiply the two-body term by an adjustable parameter that ensures convergence of the correlation energy to the exact limit for the homogeneous electron gas. The computational cost of the proposed method is comparable to the Hartree-Fock method. Moreover, the present correlation functional does not include self-interaction terms. The performance of this functional for various atoms and molecules will be presented. [1]S. F. Boys and N. C. Handy, Proc. Roy. Soc. A, **309**, 209; **310**, 43; **310**, 63; **311**, 309 (1969). [2] N. Umezawa and T. Chikyow, Phys. Rev. A **73**, 062116 (2006).

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