New correlation factors for explicitly-correlated electronic wavefunctions

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We have investigated the correlation factors $\exp(-\zeta r_{12})$, $r_{12}\exp(-\zeta r_{12})$, $\mathrm{erf}(\zeta r_{12})$, and $r_{12}\,\mathrm{erf}(\zeta r_{12})$ in place of the linear-r_{12} term for use in explicitly-correlated electronic-structure methods. The results obtained with all of these correlation factors are significantly more accurate than those obtained with the plain correlation factor r_{12}. The correlation factor $\exp(-\zeta r_{12})$ outperforms the others.

References:

1. S. Ten-no, *Chem. Phys. Lett.* **398**, 56 (2004).

2. A. J. May, E. Valeev, R. Polly and F. R. Manby, *Phys. Chem. Chem. Phys.* **7**, 2710 (2005).

3. D. P. Tew and W. Klopper, *J. Chem. Phys.*, **123**, xxxx (2005).