Local explicit correlation methods

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The implementation of a low-order scaling LMP2-R12/2*A method is described [1]. All required integrals are obtained using robust density fitting (DF) approximations [2]. Local approximations are introduced in the DF-LMP2 [3-5] as well as in the R12 treatment. In the asymptotic limit, this leads to linear cost scaling with molectur size. The impact of these approximations on the accuracy and efficiency is demonstrated and analyzed.

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[5] R. Polly, H.-J. Werner, F. R. Manby, and Peter J. Knowles, Mol. Phys. **1**02, 2311 (2004).