Local explicitly correlated MP2 theory using pair natural orbitals

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Abstract

Localization in the framework of pair natural orbitals is explored at the explicitly correlated MP2-F12 level of theory. Our results demonstrate that very small virtual active spaces, 20-50 orbitals per significant pair, return more than 98% of the basis set limit correlation energy. The extension of pair natural orbital ideas to the complementary auxiliary basis set for the RI also affords enormous truncation of the auxiliary orbital space without significant loss of accuracy.