Explicitly correlated F12 theory on modern electronic structure calculations

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Since the seminal work of Hylleraas,[1,2] explicitly correlated approaches have successfully ameliorated the slow basis set convergence of the correlation energy in molecular electronic structure calculations. We shall look back on the development of the F12 theory[3–5] focusing on our contribution to the field including the rational generator approach[6] exploiting the s-/p-wave cusp conditions in conjunction with the Slater correlation factor.[7] We will also present F12 calculations of large molecules such as organic photovoltaics materials using a hybrid MPI/OpenMP implementation for massively parallel computations.[8,9]

References

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