Numerical evaluation of four-center molecular intergals for localized orbitals

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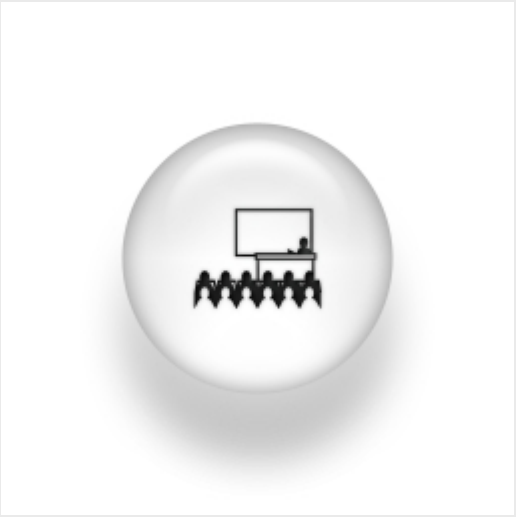

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ABSTRACT:
We have developed a computer routine to evaluate the four-center molecular integrals for the pseudo-atomic orbital basis sets.
This enables us to calculate the Fock exchange energy for Kohn-Sham orbitals within order-N DFT calculations.
In our test calculations with simple molecules, the convergence up to 10^-5 Hartree in energy has been successfully achieved at an acceptable computation cost.