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Linear scaling integral fitting ALEXANDER SODT, MARTIN HEAD-GORDON, University of California, Berkeley and LBNL Chemical Sciences Division — In density (or integral) fitting methods, the density (or an orbital product) is replaced with a sum of atom-centered "auxiliary" functions, which are used to efficiently compute Coulomb interactions. In this work, we present a method for computing localized fit coefficients that scales linearly with system size, and introduces only extremely modest errors. We apply the algorithm to a variety of methods, including the J piece of the Fock matrix.

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