Localized resolution of identity for efficient Hartree-Fock exchange, based on numeric atom-centered orbitals. JUERGEN WIEFERINK, VOLKER BLUM, XINGUO REN, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — Methods based on an exact exchange operator (EX) are increasingly popular, but are still restricted to analytical basis functions (e.g. Gaussians) for medium system sizes. We here introduce a localized resolution-of-identity approach for the two-electron Coulomb operator, based on expanding single-particle basis function products separately into auxiliary atom-centered basis sets that are restricted to two centers. Our approach produces accurate results for all-electron EX, can be applied both to analytical and numeric basis functions, requires only $O(N^2)$ intermediate storage and retains a path towards $O(N)$ EX for large systems. We demonstrate a total-energy accuracy of $<1$ meV/atom for systems including Alanine chains and the S22 benchmark molecule set [1], using the numeric atom-centered orbital based all-electron electronic structure code FHI-aims [2].


Juergen Wieferink
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

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