

Abstract Submitted  
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**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  $\mathcal{O}(N^2)$  intermediate storage and retains a path towards  $\mathcal{O}(N)$  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].

- [1] P. Jurečka *et al.*, Phys. Chem. Chem. Phys. **8**, 1985 (2006).  
[2] V. Blum *et al.*, Comput. Phys. Comm. **180**, 2175 (2009).

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