

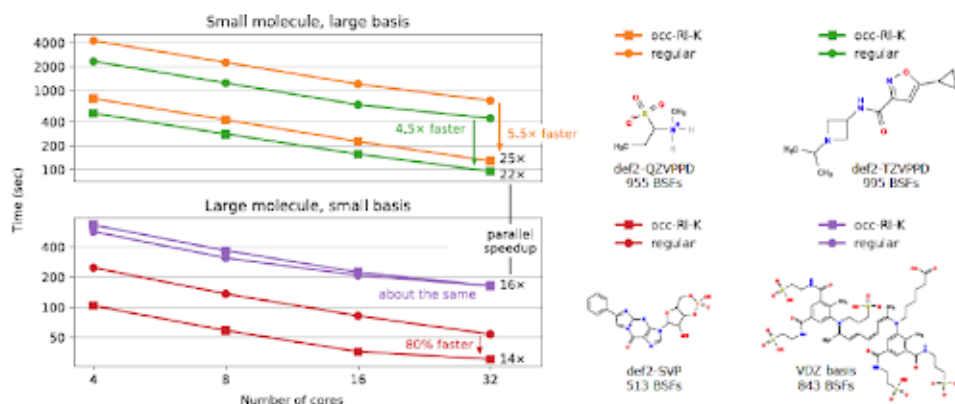
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occ-RI-K for Exact Exchange

S. Manzer, P. R. Horn, N. Mardirossian, and M. Head-Gordon, *Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm*, J. Chem. Phys. 143, 024113 (2015).

Implementation by Evgeny Epifanovsky, Joonho Lee, Fazle Rob, Samuel Manzer



Total SCF time and speedup using the occ-RI-K algorithm for evaluating exact exchange in ω B97X energy calculations. Energy computations of small molecules with large triple-zeta and quadruple-zeta quality basis sets benefit the most from the new algorithm

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