Linear-Scaling AO-MP2 for Large Systems

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A linear-scaling AO-based MP2 method is presented that allows to avoid the $\mathcal{O}(M^5)$ scaling with molecular size (M) of conventional MO-MP2 theory. We employ our multipole-based integral estimates (MBIE) for preselecting numerically significant contributions to the MP2 energy. Here, MBIE accounts for the 1/R coupling in two-electron integrals, which turns for transformed products to at least a $1/R^4$ decay behavior. While the numerical accuracy is fully preserved, we were able to calculate as largest system sofar an RNA system comprising 1664 atoms and 19 182 basis functions at the SOS-MP2 level.