Linear- and sublinear-scaling methods for describing electron-correlation effects and response properties of large molecular systems

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Progress in developing linear- and sublinear-scaling methods at density-functional theory (DFT), Møller-Plesset (MP2), symmetry-adapted perturbation theory (SAPT), and the random-phase approximation (RPA) levels is described that allows computation of molecular systems with more than 1000 atoms [1-3]. In addition, prefactors are substantially reduced using graphics processing units (GPUs) [4]. The largest MP2 calculations comprise 2025 atoms with 20 371 basis functions for protein-DNA repair complexes [2,5]. In addition, the linear-scaling calculation of response properties is discussed. For specific molecular properties such as the calculation of nuclei-selected NMR chemical shieldings, the computational effort can be reduced not only to linear, but even to sublinear (i.e., to become asymptotically independent of molecular size) [6].

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