Recent progress in *ab initio* density matrix renormalization group methodology

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We present some recent developments in the *ab initio* density matrix renormalization group (DMRG) technique for quantum chemical problems, in particular our local, quadratic scaling algorithm [1] for low dimensional systems. This method is particularly suited for the description of strong nondynamic electron correlation, and allows us to compute numerically exact correlated energies (in the sense of full configuration interaction) for large active spaces, up to one order of magnitude larger than can be treated by conventional CASSCF techniques. Other features of this method are its inherent multireference nature, i.e. it is free from the bias (and failure) of one particular configuration, its compactness of parameterization, variational results, size-consistency and size-extensivity.

In addition we will review the problems (predominantly the electronic and optical properties of organic electronic materials) on which we applied our *ab initio* DMRG algorithm, i.e.

1) metal-insulator transition in hydrogen chains [1]
2) *all-trans* polyacetylenes [1,3]
3) polyacenes [2,3]
4) polydiacetylenes [3].

Organic electronic materials share the same basic physics, namely that of conjugated π-electrons arranged in a quasi-one-dimensional network. Many properties and phenomena can be traced ultimately to the quasi-one-dimensional nature of this backbone. The strongly collective, domino-like, correlations and excitations of the π-electron system are what make these systems a serious challenge for conventional electronic structure theories. The DMRG enables us to recover the correct qualitative nature of these systems, whereas conventional MCSCF fails to capture the complete π-valence space due to the severe limitations of its exponential scaling.

[1] J. Hachmann, W. Cardoen, G.K.-L. Chan, *J. Chem. Phys.* 125 (**2006**), 144101.
[2] J. Hachmann, J.J. Dorando, M.Avilés, G.K.-L. Chan, *J. Chem. Phys.* 127 (**2007**), 134309.
[3] unpublished.