## Abstract Submitted for the MAR08 Meeting of The American Physical Society

Recent progress in ab initio density matrix renormalization group methodology JOHANNES HACHMANN, JONATHAN J. DORANDO, GARNET KIN-LIC CHAN, Cornell University — We present some recent developments in the ab initio density matrix renormalization group (DMRG) method 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 correlation, and allows us to compute numerically exact (FCI) correlated energies for large active spaces, up to one order of magnitude larger then can be done by conventional CASCI techniques. Other features of this method are its inherent multireference nature, compactness, variational results, size-consistency and size-extensivity. In addition we will review the problems (predominantly organic electronic materials) on which we applied the ab initio DMRG: 1) metalinsulator transition in hydrogen chains [1] 2) all-trans polyacetylene [1] 3) 4) polydiacetylenes [3]. References [1] Hachmann, Cardoen, Chan, acenes [2]

JCP 125 (**2006**), 144101. [2] Hachmann, Dorando, Avilés, Chan, JCP 127 (**2007**), 134309. [3] unpublished.

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