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Quadratic scaling *ab initio* DMRG for strong nondynamic correlation JOHANNES HACHMANN, WIM CARDOEN, GARNET KIN-LIC CHAN, Cornell University — We have devised a quadratic scaling *ab initio* Density Matrix Renormalization Group (DMRG) algorithm for large, linear systems (such as unbranched polymers and long molecules) [1]. It is particularly suited for the description of strong active-space nondynamic correlation. This new local method (LDMRG) is inherently multireference, compact, variational, size-consistent and size-extensive. The reduced scaling is achieved solely through integral screening and without the artificial construction of correlation domains. Due to the multireference nature of the ansatz, we also do not require restricted localization in the occupied and virtual subspaces. Numerically exact (FCI) correlated energies (in a single-zeta 1-particle basis) up to 1-10$\mu\mathrm{E}_h$ accuracy for systems with up to 100 electrons in 100 active orbitals (i.e. determinant spaces up to dimension 10^{58}) are presented. We also demonstrate the performance of the method in the study of the challenging metal-insulator transition in hydrogen-chains. We can now study nondynamic correlation in interesting classes of chemical systems, such as organic (opto-) electronic materials [2], or non-repeating chain-like molecules such as unfolded peptide backbones. [1] Hachmann, Cardoen, Chan, *JCP* 125 (**2006**), 144101. [2] Hachmann, Dorando, Avilés, Chan, *in preparation.*

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