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Abstract for an Invited Paper
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Ab-initio DMRG and Canonical Transformation Theories of Electronic Structure

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I will talk about two complementary methods that are under development in our group: (1) Ab-initio Density Matrix Renormalization Group: The Density Matrix Renormalization Group (DMRG) is a natural multireference method. Recently, we have implemented a quadratic-scaling DMRG algorithm which opens up the description of multireference (strongly interacting) correlation in large quasi-one-dimensional systems [1]. I will report calculations using this technique on conjugated oligomers correlating exactly, in the sense of Full-CI, complete pi-active spaces with up to 100 electrons in 100 orbitals (100, 100). (2) Canonical Transformation Theory: We have been developing a canonical transformation method to incorporate dynamical correlation on top of a multireference starting point. Our theory, termed Canonical Transformation Theory (CT) [2] is based on an exponential ansatz and is size-consistent. It retains the accuracy of coupled cluster theory at equilibrium bond geometries, but extends this accuracy to the full potential energy surface. The cost of the calculation is the same as for single-reference coupled cluster theory. I will report calculations using this technique for bond-breaking and excited states. I will also describe our recent efforts in developing a reduced-scaling version of the theory for large molecules. [1] J. Chem. Phys. 125, 144101 (2006) [2] J. Chem. Phys. 124, 194106 (2006)