Abstract Submitted
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Many-Body Density Matrix Theory C.J. TYMCZAK, Texas Southern University, KOSTYANTYN BORYSENKO, Boston University — We propose a novel method for obtaining an accurate correlated ground state wave function for chemical systems beyond the Hartree-Fock level of theory. This method leverages existing linear scaling methods to accurately and easily obtain the correlated wave functions. We report on the theoretical development of this methodology, which we refer to as Many Body Density Matrix Theory. This theory has many significant advantages over existing methods. One, its computational cost is equivalent to Hartree-Fock or Density Functional theory. Two it is a variational upper bound to the exact many-body ground state energy. Three, like Hartree-Fock, it has no self-interaction. Four, it is size extensive. And five, formally is scales with the complexity of the correlations that in many cases scales linearly. We show the development of this theory and give several relevant examples.

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