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Towards QMC benchmarks for large scale dispersive interactions[1]
JONATHAN L DUBOIS, RANDOLPH Q. HOOD, SEBASTIEN HAMEL, ERIC R. SCHWEGLER — Fixed-node quantum Monte-Carlo (QMC) methods are becoming an increasingly attractive approach for the study of large scale problems in electronic structure. Current challenges lie in efficient application of QMC to large (thousands of electrons) systems and removal or amelioration of the uncontrolled approximations inherent in most practical applications of the method. I will present recent progress and address some of the particular challenges associated with the development of exact potential energy surfaces for weakly interacting closed shell carbon complexes within the fixed-node QMC ansatz. In particular, the efficacy / necessity of backflow corrections and multi-determinant expansions as a method for optimizing the nodal surface in these systems will be discussed.

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