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Fragmented Molecular Orbital with Diffusion Monte Carlo for large molecular systems ANOUAR BENALI, SPENCER R. PRUITT, Argonne National Laboratory - USA, DMITRI G. FEDOROV, National Institute of Advanced Industrial Science and Technology (AIST) - Japan — Performing accurate quantum mechanics (QM) calculations on larger and larger systems, while maintaining a high level of accuracy is an ongoing effort in many ab initio fields. Many different attempts have been made to develop highly scalable and accurate methods. The fragment molecular orbital (FMO) method is an ab initio method capable of taking advantage of modern supercomputers, such as the Blue Gene Q system Mira at the Argonne National Laboratory Leadership Computing Facility (ALCF). FMO is based on dividing molecules into fragments and performing ab initio calculations on fragments, their dimers and, optionally, trimers. This decomposition makes it possible to perform QM calculations of real size biological molecules. In contrast to many other fragment-based methods, the effect of the environment is rigorously accounted for by computing the electrostatic potential (ESP) due to remaining fragments that are not explicitly included in a given monomer, dimer, or trimer calculation. The use of highly accurate levels of theory, such as Diffusion Monte Carlo (DMC-QMC), in conjunction with FMO allows for the goal of highly scalable and accurate all electron calculations demonstrated in this study, on a variety of relevant systems (H2O)[3-6] and protein using GAMESS and QMCPACK.

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