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**SILK QMC, sign-learning simulations of molecular systems**[1] XIAOYAO MA, Department of Physics and Astronomy, Louisiana State University, FRANK LOFFLER, Center for Computation and Technology, Louisiana State University, KAROL KOWALSKI, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, RANDALL HALL, Department of Natural Sciences and Mathematics, Dominican University of California, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — The Sign Learning Kink (SILK) based Quantum Monte Carlo (QMC) is used to calculate the ground state energies for $H_2O$, $N_2$ and $F_2$ molecules. This method is based on Feynman's path integral formalism and has two stages. The first, learning stage, reduces the minus sign problem by optimizing the Slater states which are used in the second, QMC stage. We test our method using different vector spaces and compare our results with other Quantum Chemical methods. We also perform exact diagonalization in those vector spaces as a benchmark. In each vector space and for each molecule, we perform SILK QMC for different bond lengths demonstrating that the SILK method is accurate for equilibrium and non-equilibrium geometries.

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