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Geometry optimization using Quantum Monte Carlo[1] LUCAS WAGNER, JEFFREY GROSSMAN, University of California, Berkeley — There are many molecular and solid systems where correlation effects need to be treated very accurately to obtain correct geometries. Current density functionals often do not perform sufficiently well in excited states, weak-binding, and transition metal oxide systems. Quantum Monte Carlo (QMC) offers very accurate total energies due to explicit treatment of electron correlation, but its stochastic nature makes precise geometry optimization challenging. We present a method that uses noisy total energies to perform a stochastic series of line minimizations. This method is efficient for multiple degrees of freedom and is effective in both the excited state and when the trial function is relatively poor–two regimes in which forces in QMC have not been developed. Details of the approach will be presented as well as a number of applications.

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