# Applications of Quantum Monte Carlo to Modeling and Simulating Transition Metal Oxides

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A fundamental problem in quantum chemistry and physics is the trade off between accuracy and speed: accurate methods frequently take too long to be practically applied to physical systems, and faster one-body methods often compromise accuracy. Quantum Monte Carlo methods are a set of stochastic processes that have shown tremendous promise in addressing this problem, able to obtain both a high accuracy, as well as being easily scalable to larger physical systems. We study applications of Quantum Monte Carlo to modeling and simulating transition metal oxides. One difficulty that arises when attempting to use typical deterministic methods or one-body theories to model transition metal oxides is that the *d*- and *f*- orbitals that are characteristic of these compounds are extremely degenerate and drastically decrease the effectiveness of standard techniques. We use Quantum Monte Carlo methods to simulate the electrons in transition metal oxides and discuss further applications of our Quantum Monte Carlo technique to simulate more general transition metal compounds. Furthermore, we test our simulations with various conditions, including phase transitions under high temperature and pressure scenarios. We subsequently compare the accuracy and speed of our Quantum Monte Carlo based simulation to those in the literature which are based on Coupled Cluster Theory, a standard deterministic method which, while extremely accurate, requires extensive time and computational power. To conclude, we discuss possible future work and our current progress on studying the corresponding wave functions of our Quantum Monte Carlo simulations.

## References

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