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Challenges for large scale ab initio Quantum Monte Carlo[1]

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Ab initio Quantum Monte Carlo is an electronic structure method that is highly accurate, well suited to large scale computation, and potentially systematically improvable in accuracy. Due to increases in computer power, the method has been applied to systems where established electronic structure methods have difficulty reaching the accuracies desired to inform experiment without empiricism, a necessary step in the design of materials and a helpful step in the improvement of cheaper and less accurate methods. Recent applications include accurate phase diagrams of simple materials through to phenomena in transition metal oxides. Nevertheless there remain significant challenges to achieving a methodology that is robust and systematically improvable in practice, as well as capable of exploiting the latest generation of high-performance computers. In this talk I will describe the current state of the art, recent applications, and several significant challenges for continued improvement.

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