New applications of Diffusion Quantum Monte Carlo

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First principles many-body Quantum Monte Carlo (QMC) methods enable the accurate prediction of electronic structure and offer an increasingly accessible alternative to density functional based methods. However, the applications of QMC have long been restricted to relatively light elements and small systems due to the computational cost. Recently the method is seeing much wider application due to both methodological developments and increased computational power. In this presentation I will discuss the materials and properties that are accessible today, as well as the achievable accuracies. I will give examples from van der Waals systems[1], metal oxides[2,3], and metallic systems relevant for catalysis, and will also outline the opportunities and prospects for reducing the remaining systematic errors in the methodology.

[1] ”Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods”, P. Ganesh, J. Kim, C. Park, M. Yoon, F. A. Reboredo, and P. R. C. Kent. Journal of Chemical Theory and Computation 10 5318 (2014). http://dx.doi.org/10.1021/ct500617z

[2] “Ab initio quantum Monte Carlo calculations of spin superexchange in cuprates: the benchmarking case of Ca2CuO3”. K. Foyevtsova, J. T. Krogel, J. Kim, P. R. C. Kent, E. Dagotto, and F. A. Reboredo. Physical Review X 4 031003 (2014). http://dx.doi.org/10.1103/PhysRevX.4.031003

[3] “Structural stability and defect energetics of ZnO from diffusion quantum Monte Carlo”, J. A. Santana, J. T. Krogel, J. Kim, P. R. C. Kent, and F. A. Reboredo. Journal of Chemical Physics 142 164705 (2015). http://dx.doi.org/10.1063/1.4919242