Abstract Submitted for the SES08 Meeting of The American Physical Society

QMC Goes BOINC: Using Public Resource Computing to Perform Quantum Monte Carlo Calculations¹ CAMERON RAINEY, LARRY ENGELHARDT, Francis Marion University, Florence, SC, CHRISTIAN SCHRÖDER, THOMAS HILBIG, University of Applied Sciences Bielefeld, Bielefeld, Germany — Theoretical modeling of magnetic molecules traditionally involves the diagonalization of quantum Hamiltonian matrices. However, as the complexity of these molecules increases, the matrices become so large that this process becomes unusable. An additional challenge to this modeling is that many repetitive calculations must be performed, further increasing the need for computing power.² Both of these obstacles can be overcome by using a quantum Monte Carlo (QMC) method and a distributed computing project. We have recently implemented a QMC method within the Spinhenge@home^{3,4} project, which is a Public Resource Computing (PRC) project where private citizens allow part-time usage of their PCs for scientific computing. The use of PRC for scientific computing will be described in detail, as well as how you can contribute to the project.

¹Funding was provided by the FMU quality enhancement plan.

²See, e.g., L. Engelhardt, et. al., Angew. Chem. Int. Ed. 47, 924 (2008).

³C. Schröder, in Distributed & Grid Computing - Science Made Transparent for Everyone. Principles, Applications and Supporting Communities. (Weber, M.H.W., ed., 2008).

⁴Project URL: http://spin.fh-bielefeld.de

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