

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Systematically improvable auxiliary-field quantum Monte Carlo for strongly correlated systems**<sup>1</sup> WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, College of William and Mary, Williamsburg, VA — The quest for an accurate and scalable many-body method for strongly correlated systems is still ongoing despite many years of efforts. The auxiliary-field quantum Monte Carlo (AFQMC) method is an exact many-body method, but it suffers from a sign problem that limits its usefulness. The phaseless AFQMC (ph-AFQMC) has been introduced<sup>2</sup> to control the sign problem. In this work we employ the unconstrained (exact) AFQMC method on massively parallel supercomputers to systematically improve ph-AFQMC results. Applications to strongly correlated systems, including transition-metal compounds, will be presented.

<sup>1</sup>Supported by DOE, ONR, and NSF. Calculations were performed at OLCF Titan and CPD.

<sup>2</sup>Zhang and Krakauer, Phys. Rev. Lett. 90, 136401 (2003)

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Date submitted: 09 Nov 2012

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