Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Hybrid quantum-classical approach to correlated materials BELA BAUER, DAVE WECKER, Microsoft Research, ANDREW J. MILLIS, Columbia University, MATTHEW B. HASTINGS, Microsoft Research, MATTHIAS TROYER, ETH Zurich — Recent improvements in control of quantum systems make it seem feasible to finally build a programmable general-purpose quantum computer within a decade. While it has been shown that such a quantum computer can in principle solve certain small electronic structure problems and idealized model Hamiltonians, the highly relevant problem of directly solving a complex correlated material appears to require a prohibitive amount of resources. Here, we show that by using a hybrid quantum-classical algorithm that incorporates the power of a small quantum computer into a framework of classical embedding algorithms, the electronic structure of complex correlated materials can be efficiently tackled using a quantum computer. In our approach, the quantum computer solves a small effective quantum impurity problem that is self-consistently determined via a feedback loop between the quantum and classical computation. Use of a quantum computer enables much larger and more accurate simulations than with any known classical algorithm, and will allow many open questions in quantum materials to be resolved once a small quantum computer with around one hundred logical qubits becomes available.

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Date submitted: 05 Nov 2015 Electronic form version 1.4