

Abstract Submitted
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The Quantum Monte Carlo Database: towards high-accuracy and high-throughput calculation of material properties JOSHUA SCHILLER, University of Illinois at Urbana-Champaign, RAYMOND PLANTE, National Institute of Standards and Technology, LUCAS WAGNER, ELIF ERTEKIN, University of Illinois at Urbana-Champaign — Quantum Monte Carlo (QMC) techniques comprise a class of promising methods that offer a path towards higher accuracy for materials property prediction. However, their application in bulk materials has historically been limited to one-at-a-time evaluation of a given material. While these results often provide benchmark-level accuracy for quantities of interest, they do not allow for high-throughput analysis of the data since each calculation is done slightly differently. We present a combined data format and automatic generation platform based on the QWalk code for QMC data: QMCDB. This platform collects QMC results and provenance information automatically and stores the information in a database. We will report on the construction of this database and what lessons can be learned about using QMC for high-throughput applications.

Joshua Schiller
University of Illinois at Urbana-Champaign

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