**QMCPACK: Predictive and systematically improvable quantum-mechanics based simulations of materials**

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**Abstract**

QMCPACK is an open source quantum Monte Carlo package for ab initio electronic structure calculations. It supports calculations of metallic and insulating solids, molecules, atoms, and some model Hamiltonians. Implemented real space quantum Monte Carlo algorithms include variational, diffusion, and reptation Monte Carlo. QMCPACK uses Slater–Jastrow type trial wavefunctions in conjunction with a sophisticated optimizer capable of optimizing tens of thousands of parameters. The orbital space auxiliary-field quantum Monte Carlo method is also implemented, enabling cross validation between different highly accurate methods. The code is speciacally optimized for calculations with large numbers of electrons on the latest high performance computing architectures, including multicore central processing unit and graphical processing unit systems. The package is available at <http://qmcpack.org>.  QMCPACK activities at ORNL are supported by the Center for Predictive Simulation of Functional Materials, a BES Computational Materials Sciences Center, and a ASCR ECP Applications Development project.