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Peta-scale QMC simulations on DOE leadership computing facilities JEONGNIM KIM, Oak Ridge National Laboratory, AB INITIO NETWORK COLLABORATION[1] — Continuum quantum Monte Carlo (QMC) has proved to be an invaluable tool for predicting the properties of matter from fundamental principles. Even with numerous innovations in methods, algorithms and codes, [2] QMC simulations of realistic problems of 1000s and more electrons are demanding, requiring millions of core hours to achieve the target chemical accuracy. The multiple forms of parallelism afforded by QMC algorithms and high compute-to-communication ratio make them ideal candidates for acceleration in the multi/many-core paradigm. We have ported and tuned QMCPACK to recently deployed DOE doca-petaflop systems, Titan (Cray XK7 CPU/GPGPU) and Mira (IBM Blue Gene/Q). The efficiency gains through improved algorithms and architecture-specific tuning and, most importantly, the vast increase in computing powers have opened up opportunities to apply QMC at unprecedent scales, accuracy and time-to-solution. We present large-scale QMC simulations to study energetics of layered materials where vdW interactions play critical roles.

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[2]Kim et al., J. Phys.: Conf. Ser., **402** 012008 (2012).

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