Abstract Submitted
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Quantum Monte Carlo Simulation of condensed van der Waals Systems[1] ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories, NICHOLS A. ROMERO, Argonne National Laboratory, JEONGNIM KIM, Oak Ridge National Laboratory, O. ANATOLE VON LILIENFELD, Argonne National Laboratory — Van der Waals forces are as ubiquitous as infamous. While post-Hartree-Fock methods enable accurate estimates of these forces in molecules and clusters, they remain elusive for dealing with many-electron condensed phase systems. We present Quantum Monte Carlo [1,2] results for condensed van der Waals systems. Interatomic many-body contributions to cohesive energies and bulk modulus will be discussed. Numerical evidence is presented for crystals of rare gas atoms, and compared to experiments and methods [3]. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DoE's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] J. Kim, K. Esler, J. McMinis and D. Ceperley, SciDAC 2010, J. of Physics: Conference series, Chattanooga, Tennessee, July 11 2011
[2] QMCPACK simulation suite, http://qmcpack.cmscc.org (unpublished)
[3] O. A. von Lillienfeld and A. Tkatchenko, J. Chem. Phys. 132 234109 (2010)

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