

# Quantum Monte Carlo for accurate predictions of correlated electronic systems

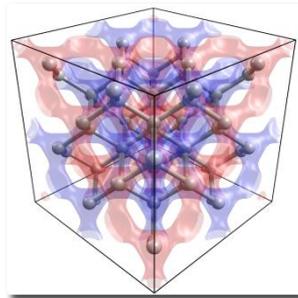
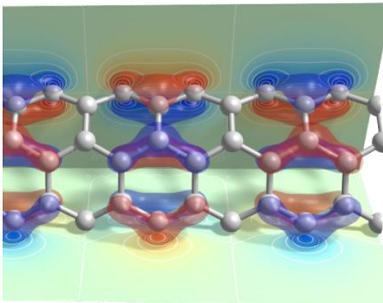
J. Kim, NCSA, Univ. Illinois

- Quantum Monte Carlo simulations for accurate predictions of correlated electronic systems
  - Exploit GPUs for large-scale, high throughput, QMC calculations
  - “Fully accelerating QMC simulations of real materials on GPU clusters”, Esler, Kim, Shulenburger & Ceperley, CISE (2010).
  - QMCPACK, <http://qmcpack.cmscc.org/>

- QMC on GPUs
  - Accelerated by many threads, high floating-point performance, and bandwidth
  - Restructure the algorithm and data structure to expose parallelism
  - MPI for load balancing & reductions
  - Main GPU kernels in single-precision

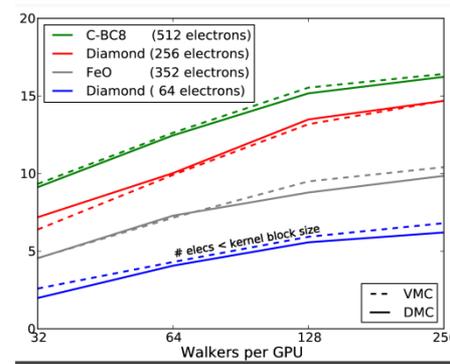
Get accurate answers, faster

- First principles calculations of molecular and solid-state systems



Esler et al. PRL (2010)

- Performance of 1 GPU ~ 30 CPU cores



Speedup of  
C1060/Quad Xeon  
E5410  
CPU: double  
GPU: mixed

NCSA Lincoln Cluster