Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation[1] LIN LIN, Lawrence Berkeley Natl Lab, GEORG HUHS, Barcelona Supercomputing Center, ALBERTO GARCIA, Institut de Ciencia de Materials de Barcelona, CHAO YANG, Lawrence Berkeley Natl Lab — We describe how to combine the pole expansion and selected inversion (PEXSI) technique with the SIESTA method, which uses numerical atomic orbitals for Kohn-Sham density functional theory (KSDFT) calculations. The PEXSI technique can efficiently utilize the sparsity pattern of the Hamiltonian matrix and the overlap matrix generated from codes such as SIESTA, and solves KSDFT without using cubic scaling matrix diagonalization procedure. The complexity of PEXSI scales at most quadratically with respect to the system size, and the accuracy is comparable to that obtained from full diagonalization. One distinct feature of PEXSI is that it achieves low order scaling without using the near-sightedness property and can be therefore applied to metals as well as insulators and semiconductors, at room temperature or even lower temperature. The PEXSI method is highly scalable, and the recently developed massively parallel PEXSI technique can make efficient usage of 10,000$\sim$100,000 processors on high performance machines. We demonstrate the performance the SIESTA-PEXSI method using several examples for large scale electronic structure calculation including long DNA chain and graphene-like structures with more than 20000 atoms.

[1]Funded by Luis Alvarez fellowship in LBNL, and DOE SciDAC project in partnership with BES.

Lin Lin
Lawrence Berkeley Natl Lab

Date submitted: 13 Nov 2013 Electronic form version 1.4