Abstract Submitted
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Hybrid MPI/OpenMP First Principles Materials Science Codes for Intel Xeon Phi (MIC) based HPC: The Petascale and Beyond[1] ANDREW CANNING, Lawrence Berkeley National Laboratory and University of California, Davis, JACK DESLIPPE, Lawrence Berkeley National Laboratory, JAMES CHELIKOWSKY, University of Texas at Austin, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Exploiting the full potential of present petascale and future exascale supercomputers based on many core chips requires a high level of threading on the node as well as reduced communications between the nodes to scale to large node counts. We will present results for a variety of first principles materials science codes (Berkeley-GW, PARATEC, PARSEC) on Intel Xeon Phi (MIC) based supercomputers for algorithms using hybrid OpenMP/MPI parallelism to obtain both efficiently threaded single chip performance and parallel scaling to large node counts.

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Andrew Canning
Lawrence Berkeley National Laboratory and University of California, Davis

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