

Abstract Submitted
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Quantum Chemistry on Petascale Machines: Done! What's Next?¹ EDOARDO APRA, Pacific Northwest Natl Lab — We will illustrate some recent application of parallel code NWChem on Petascale hardware related to material science topics. For example, we will report of the use of embedded cluster approach to model the ground state and excited state properties of crystalline compounds. The methods analyzed in the talk will range from Density-Functional based to wave-function based (e.g. Coupled Cluster). In the second half of the talk we will describe on-going software and algorithmic developments geared towards exploiting the aggregate resources available in upcoming 100 petaflops architectures.

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