

MAR17-2016-020354

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Here and now: the intersection of computational science, quantum-mechanical simulations, and materials science.

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The last 30 years have seen the steady and exhilarating development of powerful quantum-simulation engines for extended systems, dedicated to the solution of the Kohn-Sham equations of density-functional theory, often augmented by density-functional perturbation theory, many-body perturbation theory, time-dependent density-functional theory, dynamical mean-field theory, and quantum Monte Carlo. Their implementation on massively parallel architectures, now leveraging also GPUs and accelerators, has started a massive effort in the prediction from first principles of many or of complex materials properties, leading the way to the exascale through the combination of HPC (high-performance computing) and HTC (high-throughput computing). Challenges and opportunities abound: complementing hardware and software investments and design; developing the materials' informatics infrastructure needed to encode knowledge into complex protocols and workflows of calculations; managing and curating data; resisting the complacency that we have already reached the predictive accuracy needed for materials design, or a robust level of verification of the different quantum engines. In this talk I will provide an overview of these challenges, with the ultimate prize being the computational understanding, prediction, and design of properties and performance for novel or complex materials and devices.