Nanomaterials to Warm Dense Matter from First Principles

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Abstract: Over the course of the past few decades, quantum mechanical calculations based on Kohn–Sham density functional theory (DFT) have become a cornerstone of materials and chemical sciences research by virtue of the predictive power and fundamental insights they provide. However, such calculations are associated with significant computational cost, which has restricted the range of systems that can be subject to such a first-principles investigation. In this talk, the speaker will discuss efforts to overcome these bottlenecks, including large-scale parallel formulations of DFT, cyclic and helical symmetry-adapted formulations of DFT, linear scaling formulation of DFT, and machine-learning techniques to accelerate molecular dynamics simulations. The speaker will also discuss the applications that have been enabled through these efforts, ranging from those in nanoscience to those in warm dense matter.