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Challenges and advances in large-scale DFT calculations on GPUs

HEATHER KULIK, MIT — Recent advances in reformulating electronic structure algorithms for stream processors such as graphical processing units have made DFT calculations on systems comprising up to $O(10^3)$ atoms feasible. Simulations on such systems that previously required half a week on traditional processors can now be completed in only half an hour. Here, we leverage these GPU-accelerated quantum chemistry methods to investigate large-scale quantum mechanical features in protein structure, mechanochemical depolymerization, and the nucleation and growth of heterogeneous nanoparticle structures. In each case, large-scale and rapid evaluation of electronic structure properties is critical for unearthing previously poorly understood properties and mechanistic features of these systems. We will also discuss outstanding challenges in the use of Gaussian localized-basis-set codes on GPUs pertaining to limitations in basis set size and how we circumvent such challenges to computational efficiency with systematic, physics-based error corrections to basis set incompleteness.

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