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Accuracy, Speed, Scalability: the Challenges of Large-Scale DFT Simulations[1]

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First-Principles Molecular Dynamics (FPMD) simulations based on Density Functional Theory (DFT) have become popular in investigations of electronic and structural properties of liquids and solids. The current upsurge in available computing resources enables simulations of larger and more complex systems, such as solvated ions or defects in crystalline solids. The high cost of FPMD simulations however still strongly limits the size of feasible simulations, in particular when using hybrid-DFT approximations. In addition, the simulation times needed to extract statistically meaningful quantities also grows with system size, which puts a premium on scalable implementations. We discuss recent research in the design and implementation of scalable FPMD algorithms, with emphasis on controlled-accuracy approximations and accurate hybrid-DFT molecular dynamics simulations, using examples of applications to materials science and chemistry.

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