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Multi-petaflop/s quantum and reactive molecular dynamics simulations

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We have developed a divide-conquer-recombine algorithmic framework for large quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations. The algorithms have achieved parallel efficiency over 0.98 on 786,432 IBM Blue Gene/Q processors for 39.8 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 67.6 billion-atom RMD. We will discuss several applications including (1) 16,616-atom QMD simulation of rapid hydrogen production from water using metallic alloy nanoparticles, (2) 6,400-atom nonadiabatic QMD simulation of exciton dynamics for efficient solar cells, and (3) 112 million-atom RMD simulation of nanocarbon synthesis by high temperature oxidation of SiC nanoparticles.