**Periodic DFT calculations of vibrational and molecular dynamics of large systems using OLCF computers**

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**Abstract**

Density functional theory (DFT) calculations on increasingly large systems have become possible in recent years with HPC-based parallel programs. Time-to-solution and scaling benchmarks for both vibrational normal mode calculations and molecular dynamics simulations using the periodic VASP and CP2K programs are presented. Accuracy of vibrational calculations is assessed using comparisons to incoherent neutron vibrational spectra collected on the VISION instrument at SNS. The first ab initio molecular dynamics (AIMD) simulations of fully solvated small biomolecules using the linear-scaling SCF routine in CP2K is also presented, and results are compared to classical molecular dynamics simulations. We show the possibility of AIMD as a new tool for biomolecular simulation with this increasing performance on HPC systems.