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Stochastic vector computational approaches to finite temperature DFT and electronic structure of large systems

Monday 21 February 2022 14:00 (1 hour)

Stochastic vector computational approaches for the electronic structure of extended condensed matter systems help reduce algorithmic complexity, facilitate efficient parallelization, simplify computational tasks, accelerate calculations, and diminish memory requirements. The electronic density is estimated by a stochastic process that samples the Kohn-Sham eigenstate contribution according to the Fermi Dirac occupation, completely avoiding the actual calculation of eigenstates. The method is expected to be especially useful for finite-temperature density functional-based molecular dynamics calculations. We also discuss the use of stochastic approaches for estimating quasiparticle energies within the G0W0 approximaiton.

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