Hartree Centre
Science & Technology Facilities Council

CP2K: Highly scalable atomistic simulation for all

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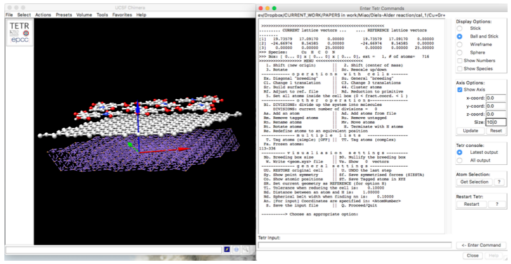
Open-source, flexible atomistic simulation code:

- QUICKSTEP DFT
- Fast Hybrids (ADMM)
- Linear Scaling DFT
- Post-HF: MP2, RPA, GW
- Time-Dependent DFT
- Electronic Transport (NEGF)

Scalability & HPC focus:

- Gordon Bell Nominee 2015
- Sparse Matrix Algebra DBCSR
- MPI + OpenMP parallel
- CUDA kernels / OpenMP
- Xeon Phi KNL
- Single-sided MPI RDMA
- Auto-tuned JIT kernels (libxsmm)

Coupled to a range of community tools:



Training and support available via CP2K-UK project:

CP2K Summer School 2018
19-22 June, Hartree Centre,
Sci-Tech Daresbury

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