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FFTW 3.3.7

/fs00/software/fftw/3.3.7-iccifort-17.0.6-* □□ iccifort/17.0.6

FFTW 3.3.8

/fs00/software/fftw/3.3.8-ips2019u5 □□ ips/2019u5

LAMMPS 11Aug17

/fs00/software/lammps/11Aug17

LAMMPS 23Jun2022

/fs00/software/lammps/23Jun2022

LAMMPS 22Jul2025

/fs00/software/lammps/22Jul2025

OpenFOAM® v1806

/fs00/software/openfoam/v1806-ips2017u6

source /fs00/software/openfoam/v1806-ips2017u6/OpenFOAM-v1806/etc/bashrc

P4vasp 0.3.29

/fs00/software/p4vasp/0.3.29

Modulefile: p4vasp/0.3.29

Phonopy 1.11.2

/fs00/software/phonopy/1.11.2

Quantum ESPRESSO 5.2.0 & 6.1

/fs00/software/qe/5.2.0-ips2015u3/ □□ ips/2015u3

/fs00/software/qe/6.1-ips2017u2/ □□ ips/2017u2

ShengBTE

/fs00/software/shengbte □□ iccifort/15.0.3 openmpi/1.10.0-iccifort-15.0.3

Siesta 3.2-pl-5

/fs00/software/siesta/3.2-pl-5 □□ ips/2017u6

thirdorder 1.0.2 04d3f46feb78

/fs00/software/thirdorder/1.0.2

Modulefile: thirdorder/1.0.2 □□ anaconda/2-4.3.1 spglib/1.9.9

TBPLaS

/fs00/software/tbplas

MKL+MPI Version

Modulefile:

- oneapi/2024.0/compiler/2024.0.2
- oneapi/2024.0/ifort/2024.0.2
- oneapi/2024.0/mkl/2024.0
- oneapi/2024.0/mpi/2021.11

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