OOKAMI PROJECT APPLICATION

Date: April 22, 2021

Project Title: Electron-phonon coupling on a fine grid

Usage:

- Testbed

Principal Investigator:

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Names & Email of initial project users:

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Usage Description:

We will carry out the following work:

- Testing the performance of the existing code EPW. EPW code is part of the QE package and it can be compiled on ARM machines.

- Write a small program using Fortran and openmp/MPI that can read the output generated by EPW to efficiently calculate the Fourier transform of various physical quantities such as Hamiltonians, dynamical matrices and electron-phonon scattering matrices.

Computational Resources:

- Total node hours per year: 10,000

- Size (nodes) and duration (hours) for a typical batch job: One node for 72 hours.

- Disk space (home, project, scratch): home (40 GB), project (1 TB) and scratch (1 TB)

Personnel Resources:

None

Required software:

GCC, Python3.8, vim