# OOKAMI PROJECT APPLICATION

**Date:** 08/20/2021

**Project Title:** Computational design and discovery of advanced thermoelectric materials for sustaibale future energy applications

**Usage:**

☒ Testbed

☐ Production

**Principal Investigator:** Dr. Yedukondalu Neelam & Prof. John B. Parise (Supervisor)

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**Names & Email of initial project users:** Dr. Yedukondalu Neelam & yeddukondalu.neelam@stonybrook.edu

**Usage Description:** Porting and tuning VASP for A64FX and benchmarking studies on small to large scale systems

**Computational Resources:**

Total node hours per year: less than 15k hours per year

Size (nodes) and duration (hours) for a typical batch job: 1-2 weeks long with 40-cores per node

Disk space (home, project, scratch): home: 20-40GB, Project: 5 TB storage

**Personnel Resources (**assistance in porting/tuning, or training for your users**):** Training for VASP and USPEX users

**Required software: VASP, USPEX, TDEP**

**If your research is supported by US federal agencies:**

Agency:

Grant number(s):