

# OOKAMI PROJECT APPLICATION

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**Date:** 13/11/2021

**Project Title:** Testing and benchmarking electronic structure calculations code VASP on OOKAMI platform

**Usage:**

Testbed

Production

**Principal Investigator:**

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**Names & Email of initial project users:**

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**Usage Description:**

The allocation is requested to investigate portability of VASP code, assess its performance on the system, and tune performance of the code with particular emphasis on issues related to parallelization.

**Computational Resources:**

Total node hours per year: 15,000 node-hours

Size (nodes) and duration (hours) for a typical batch job: 4 nodes/48 hours

Disk space (home, project, scratch): 20GB/500GB/500GB

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

Need assistance in porting VASP

**Required software:** VASP (<https://www.vasp.at/>)

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

Agency: The Office of Naval Research

Grant number(s): Award number: N00014-20-1-2231

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**Production projects:**

Production projects should provide an additional 1-2 pages of documentation about how  
(a) the code has been tuned to perform well on A64FX (ideally including benchmark data comparing performance with other architectures such as x86 or GPUs)

(b) it can make effective use of the key A64FX architectural features (notably SVE, the high-bandwidth memory, and NUMA characteristics)

(c) it can accomplish the scientific objectives within the available 32 Gbyte memory per node