OOKAMI PROJECT APPLICATION

Date: June 30, 2022

Project Title: Study on the Influence and Mechanism of Moiré Patterns on Lattice Thermal Conductivity of Bilayer WS_2 via First-Principles Calculation

Usage:

☒ Testbed

☐ Production

Principal Investigator:

University/Company/Institute:	Stevens Institute of Technology
Mailing address including country:	Annie Xian Zhang, 407 Edwin A. Stevens Hall, 24 5th Street, Hoboken, NJ, US, 07030.
Phone number:	(201) 216-5386
Email:	xzhang4@stevens.edu
Names & Email of initial project users:	Yingtao Wang ywang414@stevens.edu

Usage Description: These computation resources will be used to test the size and scale performance of our codes in order to provide the scale performance report to apply to ookami research projects. In future formal research, we will perform theoretical simulations to calculate the thermal conductivity of bilayer WS_2 through density functional theory (DFT) mounted in the VASP package by solving the Phonon Boltzmann transport equations (BTE). The thermal conductivity under several twist angles and the influence law of Moiré patterns on thermal conductivity will be summarized. A reasonable mechanism explanation will also be given. A rational experiment is further set up to verify the rationality of the mechanism.

Computational Resources:

Total node hours per year: 1000 node hours

Size (nodes) and duration (hours) for a typical batch job: About 8 nodes 2 hours

Disk space (home, project, scratch): the sizes of our input and output files are small, so 10 GB is enough.

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

Required software: Vienna Ab initio Simulation Package (VASP)

If your research is supported by US federal agencies:

Agency:

Grant number(s):

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