



Contribution ID : 45

Type : MCRP-S

Development of combined machine learning potential and molecular mechanics force field (MLP/MM) method and its applications

Email

kiyoshi.yagi@chem.tsukuba.ac.jp

Number of project members

1

Pegasus/Sirius: Project code

qmmm-dev [QMMMDEV]

Node-hour product for Pegasus

5000 [2940]

Pegasus: Requested disk capacity (TB)

[3]

Pegasus: Disk larger than the standard value?

No

Node-hour product for Sirius

[0]

Sirius: Requested disk capacity (TB)

[0]

Sirius: Disk larger than the standard value?

No

Miyabi project code

None [xg26i045]

Node-hour product for Miyabi-G

15000 [12960]

Node-hour product for Miyabi-C

2000 [1920]

Miyabi: Requested disk capacity (TB)

[1]

Miyabi: Disk larger than the standard value?

No

Have UTID-13 ?

Yes, I have UTID-13.

UTID-13

0000299150042

Primary author(s) : YAGI, Kiyoshi

Track Classification : Chemistry(化学分野)