Contribution ID : 50   Type : MCRP-M

Exploring performance of DFT-MD simulation for interfacial water

Number of project members

2

Cygnus: Project code

DFTMDPER [非採択]

Cygnus: Requested [awarded] number of nodes

Cygnus: Requested [awarded] node-hour product

Cygnus: Requested [awarded] disk capacity (TB)

15 [0]

OFP: Project code

DFTMDPER [xg19i050]

OFP: Requested [awarded] number of nodes

2048 [1024]

OFP: Requested [awarded] node-hour product

1000000 [210000]

OFP: Requested [awarded] disk capacity (TB)

20 [20]

Primary author(s) :   Dr NAGATA, Yuki (Max Planck Institute for Polymer Research)

Co-author(s) :   Dr OHTO, Tatsuhiko (Graduate School of Engineering Science, Osaka University)

Track Classification :   Chemistry（化学分野）