Usage Report for Fiscal Year 2020

Project Title:

Evaluation of Electronic Structure and Excited State Dynamics of Metal Complexes

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1. If no job was executed, specify the reason.

I tried to use OpenMolcas, which is one of quantum chemistry program suites, on Hokusai, but found that a few problems appeared in CASPT2 and RASSI calculations on Hokusai. Thus, I executed almost no job.