SimStack

File Run Configuration Help

Nodes

DFT-Turbomole

Untitled

DFT-Turbomole

INT-NANO Disconnect

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Follow-up calculation

Title: Title

Molecular structure

Structure file type: xyz

Structure file: structure file

Internal coordinates

Basis set

Basis set type: def2-SVP

Initial guess

Charge: 0

Multiplicity: 1

DFT options

Max SCF iterations: 2996

Use RI

Memory for RI: 1997

Functional: None

Integration grid: m3

vdW correction: None

COSMO calculation

Type of calculation

Structure optimisation

Excited states calculation

Hyperpolarizability

Frequency calculation

Plot Homo-Lumo Orbt

Workflows

pt
n-opt-sol
er-b3
er-sol-tzvp
b-b3-chcl3
b-b3-gas
p-b3-chcl3
p-b3-gas
1
0
p-1310-svp
freq
-1310-m3
-1310-m5

Controls

AdvancedFor
ForEach
If

0%