Bayesian optimization with Salmon

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Motivation

To calculate optical response of material

To know most efficient energy absorption

Calculation of optical response is expensive

Want to explore efficiently

Works

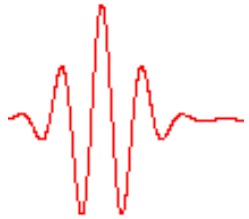
1. Pick up same parameters randomly
2. Calculate optical response with Salmon (tddft)
3. Use Bayesian optimization to determine next param

Iteration

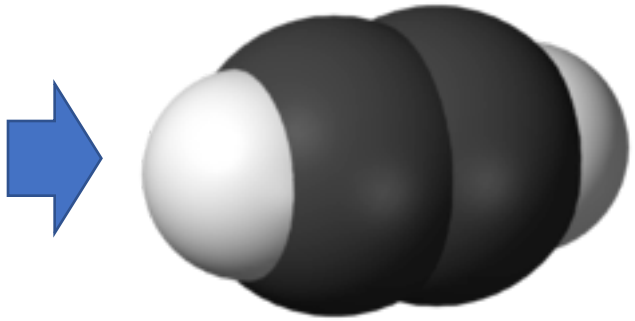
Method

Material : C_2H_2 molecule

Light 1



Light 2



Calculate Prams

Grids : 4×4×4

Functional : LDA

Light prams

$\hbar\omega_1$: 1.55 eV

$\hbar\omega_2$: 3.1 eV

T_{pulse} : 40 fs

I_1 : 0.0~2.0×10^{16} W/cm^2

$I_1 + 2I_2$ = const.

Bayesian optimization params

Combo

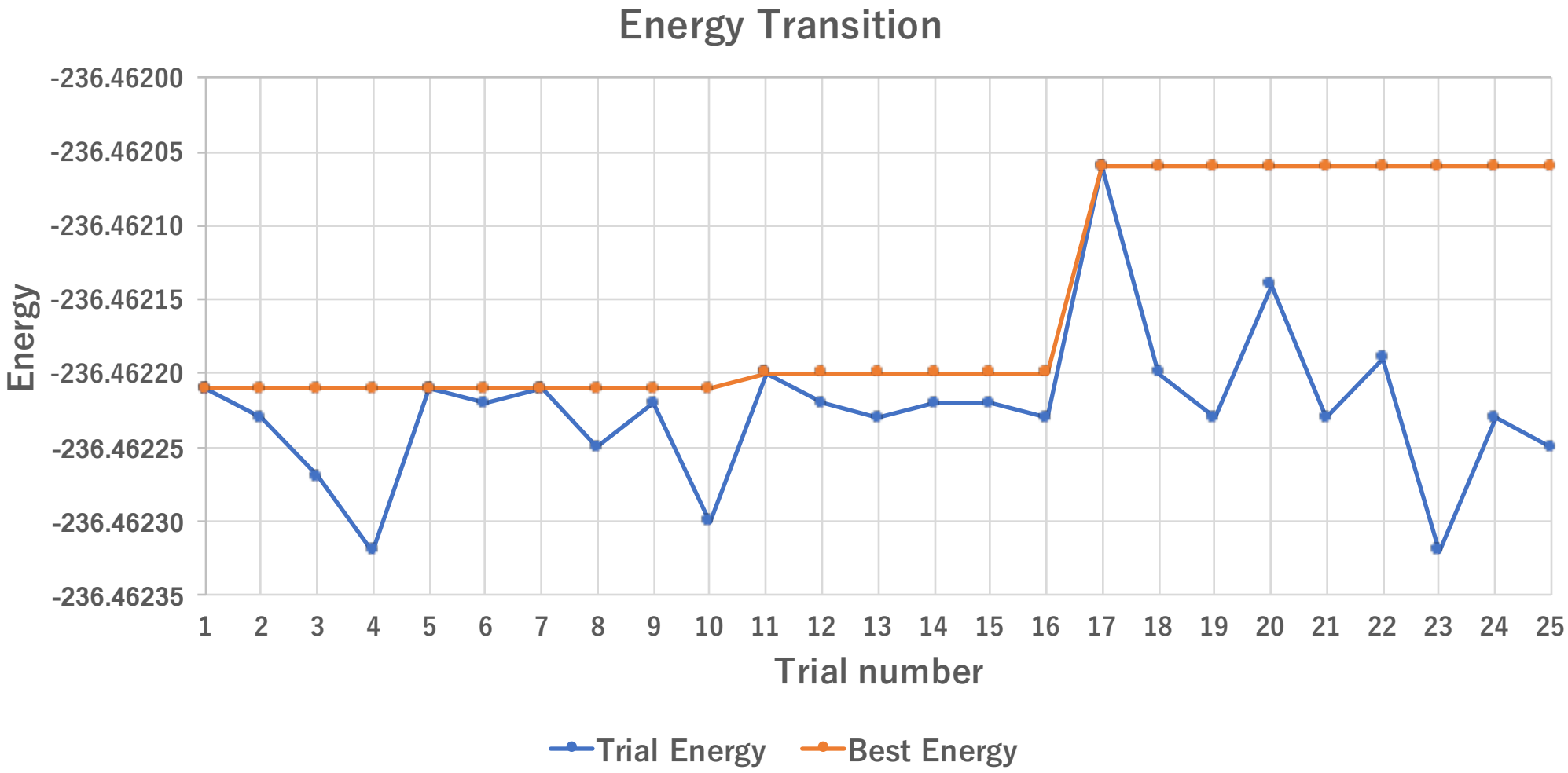
Search range : 80 (I_1 = 0.0~2.0)

Max explore : 25

Explore randomly : 5

Param tuning : every 5 iteration

Result


Energy Transition
-236.46200
-236.46205
-236.46210
-236.46215
-236.46220
-236.46225
-236.46230
-236.46235
Energy
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
Trial number
Trial Energy
Best Energy