

AITP Research Notebook

Topic:

AITP Kernel

Generated: 2026-04-18T21:01:49+08:00

目录

1 [candidate_update] Hubbard model ground-state energy estimate

Time: 2026-04-18T21:01:46+08:00 | Run: run-2026-04-18-a | Status: success

Using variational Monte Carlo on a 8x8 lattice with $U/t=4$, we obtain a ground-state energy of $E_0 = -0.87t$ per site. The result agrees with the QMC benchmark within 2%.

candidate_id cand-hubbard-gs-001

claim_type numerical_benchmark

trust_level medium

promotion_status pending

2 [strategy] Pulay mixing significantly accelerates SCF convergence for BH3 molecule

Time: 2026-04-18T21:01:47+08:00 | Run: run-2026-04-18-a | Status: helpful

Switching from simple linear mixing ($\alpha=0.3$) to Pulay mixing with history=8 reduced the SCF cycle count from 47 to 12 for the BH3 molecule in QSGW calculation.

strategy_type verification_guardrail

confidence 0.85

strategy_id strat-pulay-bh3

3 [auto_action] skill_discovery: knowledge-hub skill check

Time: 2026-04-18T21:01:48+08:00 | Run: run-2026-04-18-a | Status: completed

action_id act-skill-001

action_type skill_discovery

4 [iteration_journal] Iteration iter-003: SCF convergence confirmed

Time: 2026-04-18T21:01:49+08:00 | Run: run-2026-04-18-a | Status: success

The third iteration confirmed SCF convergence with residual $< 1e-8$. Band gap converged to 6.2 eV, consistent with the experimental value of 6.0 eV.

iteration_id iter-003

total_iterations 3

staging_decision promote

5 [closed_loop_result] Result: success —QSGW band gap for BH3

Time: 2026-04-18T21:01:49+08:00 | Run: run-2026-04-18-a | Status: success

The quasiparticle band gap was computed as:

$$E_g^{\text{QSGW}} = \langle \psi_c | \Sigma(\epsilon_c) - v_{xc} | \psi_c \rangle - \langle \psi_v | \Sigma(\epsilon_v) - v_{xc} | \psi_v \rangle$$

Result: $E_g = 6.2$ eV, compared to experimental $E_g^{\text{exp}} = 6.0$ eV. The relative error is 3.3%, within the acceptable threshold of 5%.

result_id result-qsgw-bh3-001

task_id task-band-gap-bh3

decision keep

route_id route-qsgw-numerical
