



LatticeMind
v0.5

NANOACADEMIC
TECHNOLOGIES
Coherent Modeling

+ +
+ +

AGENTIC AI PLATFORM FOR DFT SIMULATION

From natural language to material simulation results

Describe the materials problem in plain language. LatticeMind plans the workflow, builds the simulation project, runs the solvers and explains the results.

You drive the science. LatticeMind runs the simulations.

RESCU

NANODCAL

VASP

multi-package · model-agnostic

LatticeMind

1

prompt to a full validated workflow

3

DFT engines supported

5

AI model providers, incl. local

Ask in plain words. LatticeMind does the work and checks with you before anything runs.

Lattice**Mind** covers the whole loop: understanding your request, preparing inputs with built-in expert judgment, validating them against the physics, running the solver where you choose and explaining the results.

HOW LATTICEMIND WORKS



ASK A FOLLOW-UP AND IT CONTINUES FROM THE RESULTS ALREADY IN YOUR PROJECT

THE PAIN POINTS LATTICEMIND REMOVES

P · 01

Manual setup is slow

Input decks, pseudopotentials and staging are built by hand — slow and error-prone.

P · 02

Failed jobs burn budget

Trial-and-error runs waste HPC core-hours and calendar time.

P · 03

Fragmented workflow

Setup, execution and analysis live in disconnected tools.

LATTICEMIND'S CORE ADDED VALUES

Expert judgment, built in

Structures, parameters and potentials chosen as a specialist would, with every input checked by a physics validation layer.

You stay in control

Every run shows the exact command, machine and folder first. Routine runs can go ahead automatically.

Deploys with your stack

Your workstation or HPC cluster, and the AI model you choose. No lock-in.

Lower cost per result

Invalid inputs are caught before they reach the cluster. A band structure result costs about \$0.1 in AI model fees.

See exactly what's going on.

The Control room shows every part of the conversation backstage as it happens. Work seamlessly in your browser or in your terminal.

HOW THE PIECES ARE WORKING TOGETHER

1 Overview: You, your turn, Session service, Research agent, Tools, Solver, Evidence.

2 RESEARCH AGENT: provider: openai, model: gpt-5.6-luna, protocol: responses-v1, reasoning items: carried between turns, usage reporting: tokens reported, session: lm_session_52036811552f4d04a49b3a5a9a483caf, project folder: D:\research\silicon-bands.

3 CURRENT TURN: state: idle, doing: —, elapsed: —, model requests: —, tool calls: —, worker: finished · dispatch_faeac2, reason: —.

4 PERMISSIONS: answered by: you, one at a time, waiting now: nothing. Buttons: Switch on approve-for-me, 14:30:39 approved by you, 14:28:56 approved by you.

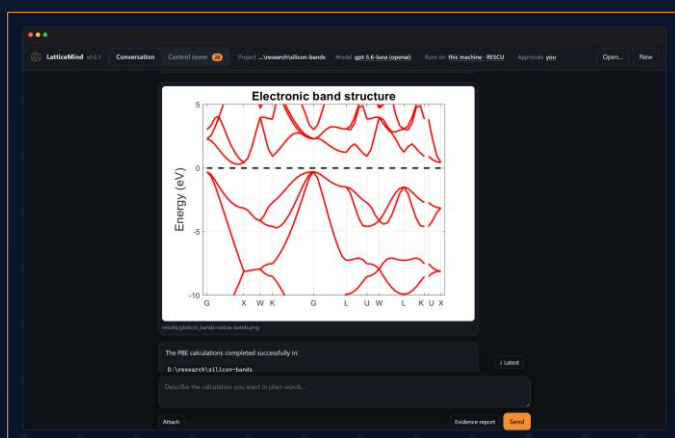
5 TOOL ACTIVITY: 20 CALLS · 14 TOOLS. Log of tool calls with timestamps and descriptions.

6 PROJECT FILES: Recently inspected or written. Lists files like results/plots/si_bands-native-spectrum.png, results/plots/si_bands-native-bands.png, D:\research\silicon-bands, project_ae4fb7b7b5dd0f18ea9230be043a1a1, rescu · D:\research\silicon-bands, asset (1), pseudopotentials/Si_PBE_TM_DZP.mat (443 KB), figure (2), results/plots/si_bands-native-bands.png (46 KB), results/plots/si_bands-native-spectrum.png (181 KB), input (2), bs.input (0 KB).

7 SOLVER RUNS: si_bands finished, rescu · run_run_82b67d22850e · 14:31:01, si_scf finished, rescu · run_run_0a46e0f47857 · 14:29:45.

THE CONTROL ROOM - model, current step, approvals, files and runs at a glance

- 1 Overview · You, the AI model, tools, solver and evidence
- 2 Research agent · the AI model in use
- 3 Current turn · what LatticeMind is doing right now
- 4 Permissions · who approves, and every answer given
- 5 Tool activity · every step, in order, with its time
- 6 Project files · every input, potential and figure
- 7 Solver runs · each run with its state and live log



THE CONVERSATION · a silicon band structure, asked for in one sentence

```
LatticeMind
LatticeMind > Run a PBE SCF for bulk silicon (two-atom diamond cell, a = 5.43 Å) and report the total en
listing structure recipes
project directory D:\research\silicon-cli
creating the project
building the structure (bulk_prototype, 2 atoms)
reading the solver reference (rescu, SCF)
searching the solver manual (5 passages)
checking a potential file (Si:PBE:DZP:Si_PBE_TM_DZP.mat)
proposing validated starting parameters
declaring calculations
binding potentials
rendering solver inputs

LatticeMind is ready to run the solver. Permission to launch?
command D:\rescu-2.9.0\bin\rescu.exe -i scf.input
on workstation (local)
in D:\research\silicon-cli\LatticeMind\runs\run_45eb89d0de1fie78b63852d0

1. yes run it this once
3. no do not run it
Answer in words (yes, go ahead, run it / no) or with a number.

LatticeMind > yes
[approved] launching

# 1 | -7.574e+00 2.403e-01 1.088e+00 1.890e+00 13:13:50
# 2 | -7.730e+00 9.858e-03 6.993e-03 5.894e-01 13:13:50
# 3 | -7.888e+00 2.632e-02 1.976e-02 6.741e-01 13:13:51
# 4 | -7.893e+00 1.551e-03 6.355e-04 4.773e-01 13:13:52
```

THE TERMINAL · the same work, with the same approval before each run

Six capabilities. One guided workflow.

Each replaces a manual stage of the simulation workflow. Together they take a question to a checked result, with expert judgment at every step.

M · 01



Plain-language requests

Start from a sentence, a paper or a structure file, and ask follow-ups in the same session.

M · 02



Built-in expert judgment

Structures, parameters and pseudopotentials chosen the way a specialist would.

M · 03



Physics validation

Units, sampling, potentials, spin and run dependencies checked against the solver's rules before any job runs.

M · 04



Run anywhere qBraid

Your workstation or HPC cluster, with the solver's own output shown live.

M · 05



Automatic analysis

Band structures, DOS, convergence checks and custom figures, read from the solver output.

M · 06



Traceable reports

Every number traced to the solver's output. The Control room shows each step, approval and run live, so you can follow and check the work.

Your DFT engine

MULTI-PACKAGE

RESCU

NANODCAL

 VASP

Native support for the solvers you already trust — commercial and community codes alike. The agent speaks each solver's input language fluently.

Your AI model

MODEL-AGNOSTIC

GPT

Claude

Gemini

Qwen

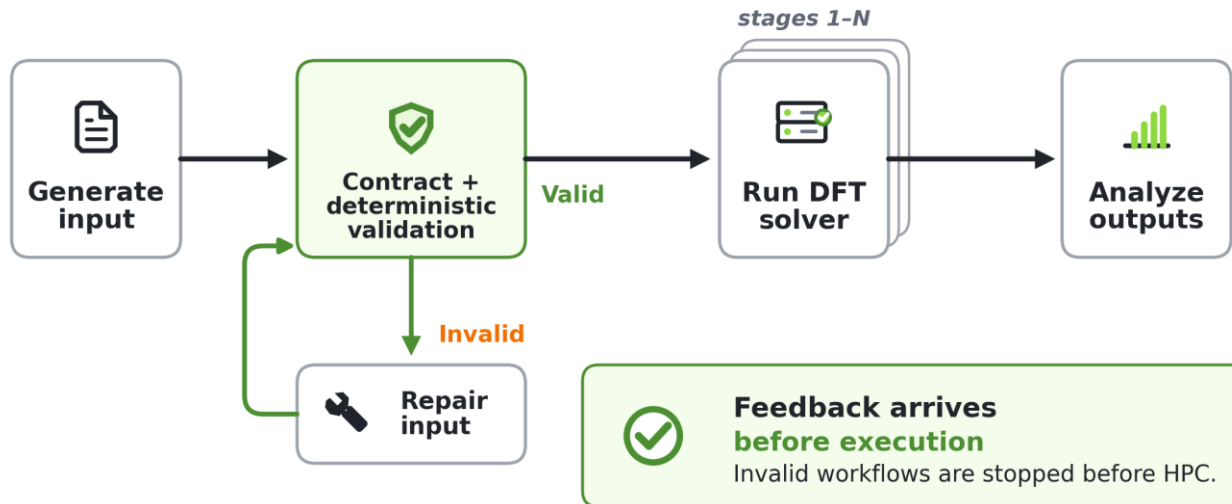
Use OpenAI, Anthropic, Google or Qwen models in the cloud, or a local model with Ollama. Accuracy comes from the architecture, not a single vendor.

INTERFACE

Browser or terminal · plain-language requests · full history, logs and figures ·
Windows, macOS and Linux

Validated by physics. Approved by you.

Built-in expert judgment proposes the setup; a physics validation layer checks every input against the solver's rules and repairs what it can. Nothing runs until you approve it.



TECHNOLOGY STACK

INTERFACE	Browser and terminal	one session, either window
AI MODEL	Reasoning + built-in expert judgment	GPT · Claude · Gemini · Qwen · local
VALIDATION	Physics validation layer	check + repair, then your approval
SOLVERS	Multi-package DFT layer	RESCU · NanoDCAL · VASP
COMPUTE	Your workstation or HPC cluster	data stays on your infrastructure

DIFFERENTIATION

■ Asks where it matters

Routine runs can go ahead; deleting files and running scripts always ask.

■ Solver- & model-agnostic

Three DFT engines and any leading AI model — cloud or local.

■ Picks up where you left off

The whole project lives in your folder; reopen it later and continue.

■ High compute utilization

Validation before execution keeps every core-hour productive.

TRUST

Physics validation · approval before every run · reproducible project folders · your data stays on your infrastructure

You decide what runs.

Choose how much LatticeMind may do without asking. Everything it produces is saved as ordinary files in the folder you started in.

APPROVALS

DEFAULT

Ask me

Every run and every change to your files is shown first — the command, the machine and the folder — and waits for your yes or no.

LatticeMind is ready to run the solver.

```
rescu -i scf.input · workstation
```

or type yes · go ahead

Answer with a button or in words, in the browser or the terminal.

OPTIONAL

Approve for me

Routine work goes ahead; anything that could lose work still asks.

GOES AHEAD

- Solver runs of low or medium cost
- New folders in the project

STILL ASKS

- Moving, copying or deleting files
- Writing into files
- Running programs and scripts
- Expensive runs, or runs of unknown size

Every automatic approval is recorded with its reason.

YOUR FOLDER IS THE PROJECT

si-bands/

← start LatticeMind here

— scf.input bs.input

The solver's own input files, ready to read or rerun by hand

— pseudopotentials/

The exact potentials each run used

— results/

Output data, figures and analysis

— .latticemind/

The session history, every run and every revision

CONTINUE

Start LatticeMind in the same folder again and it picks up where you left off, with every result in place.

APPLICATION DOMAINS

Magnetic materials

Catalysis & surfaces

Semiconductors

Quantum transport

2D materials

Battery materials

Carbon nanotubes, graphene

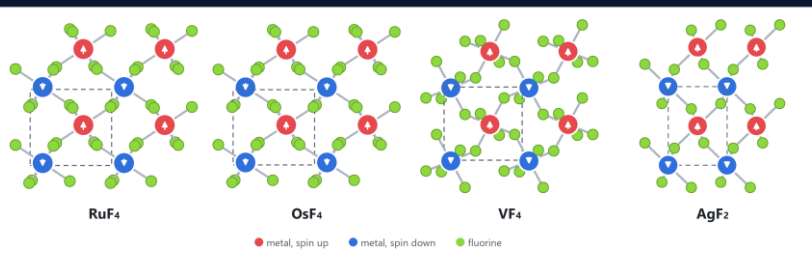
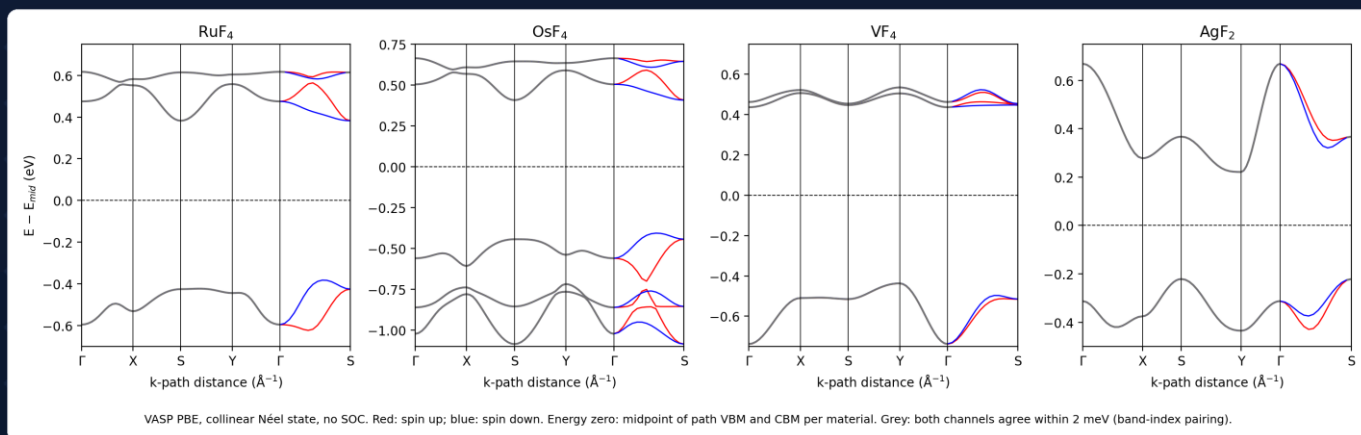
Metal alloys

Molecular devices

Nanomaterials

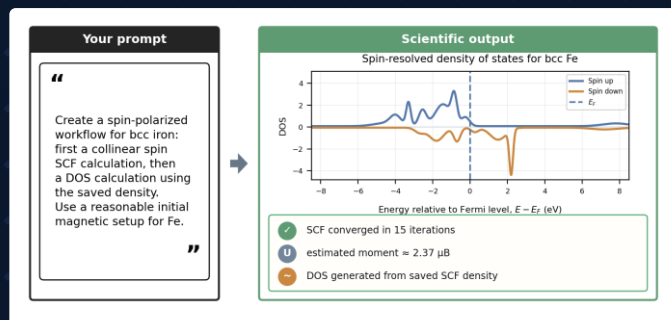
Reproducing a published result

LatticeMind read Sørdequist and Olsen, Appl. Phys. Lett. 124, 182409 (2024), ran VASP for four 2D altermagnets and redrew Fig. 1. The result matches the published figure panel for panel.

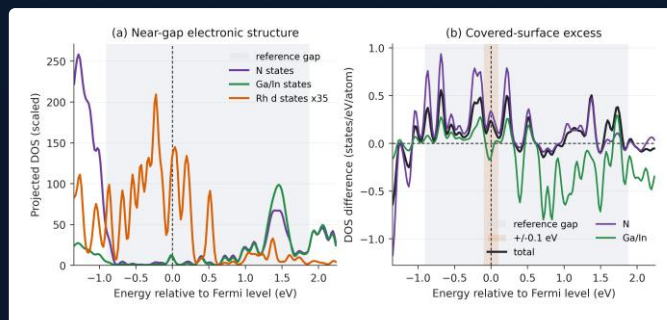


Four monolayers in their antiferromagnetic (Néel) state. Spin-up (red) and spin-down (blue) bands coincide along Γ -X-S-Y- Γ and split along Γ -S.

More case studies



One request → a spin-polarized SCF and DOS for bcc iron, run and analyzed

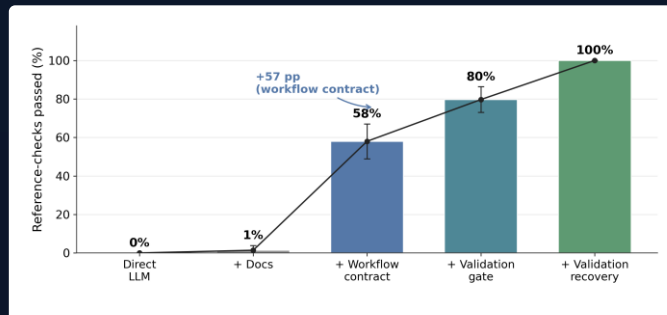


Rh-decorated GaN/InGaN photocatalyst surface – near-gap states resolved

Benchmarked reliability

On our 44-case DFT benchmark, run with three AI models, LatticeMind passed all 132 reference checks. An AI model working from the documentation alone passed 1%. Physics validation lifts the pass rate from 58% to 100%.

Checks cover workflow, structure and required physical values

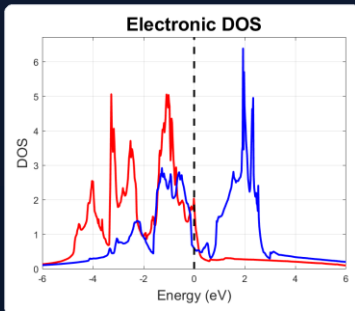


One workflow, every solver.

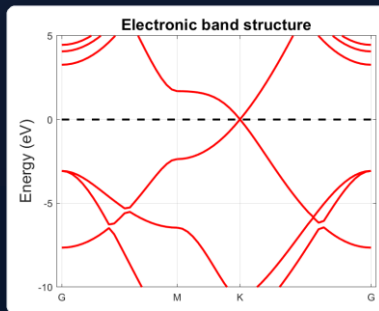
Ask the same way whichever engine you use. LatticeMind writes each solver's native input, validates it and reads the results from that solver's own output.

RESCU Magnetic, 2D and semiconductor materials

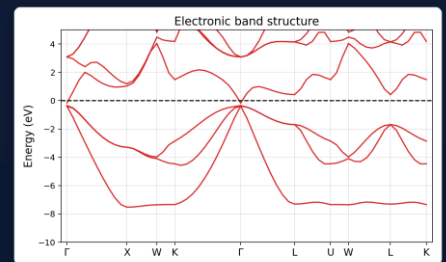
Real-space DFT for bulk crystals, surfaces and layers: spin-polarized metals, Dirac materials and semiconductors, each set up from a single sentence.



bcc Fe · 2.3 μ B per atom



Graphene · the Dirac cone at K

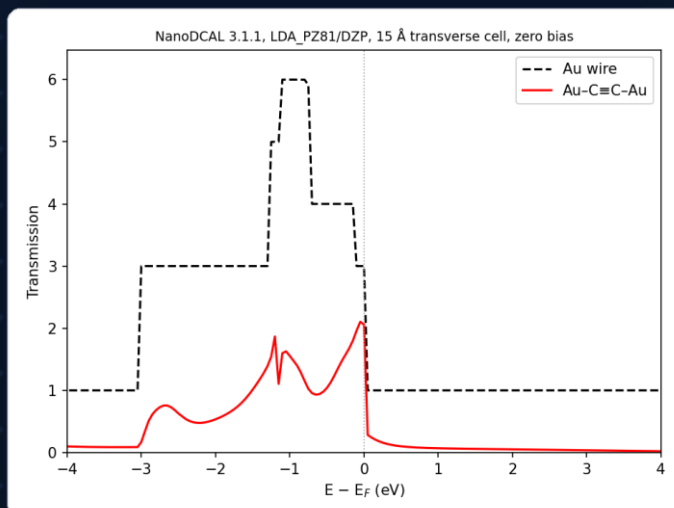


GaAs · direct gap at Γ



Quantum transport through a molecular junction

LCAO and NEGF calculations for devices and molecular junctions. LatticeMind set up a gold atomic wire and an Au-C $\equiv$ C-Au junction, a carbon triple bond bridging two gold wires, and computed their transmission.



Transmission of the gold wire (black) and the Au-C $\equiv$ C-Au junction (red), NanoDCAL LDA

The gold wire

A perfect wire carries a whole number of channels, one per band at each energy. The gold wire shows this staircase at every energy away from a band edge, up to six channels.

The molecular junction

The C $\equiv$ C bridge cuts transmission across the whole range, leaving four peaks below E_F and almost no transmission above it.

SOLVERS

RESCU · NanoDCAL · VASP – native inputs you can read and rerun, the same approval before every run



LatticeMind

Put an AI research agent on
your materials team.
Monthly & yearly subscriptions available.



SCAN FOR DEMO & DOCUMENTATION

Request a demo

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NANOACADEMIC
TECHNOLOGIES

Coherent Modeling

— FROM NATURAL LANGUAGE TO DFT RESULTS —

EVERYWHERE

ANYTIME

Windows, macOS and Linux • browser or terminal • close it any time and pick up
where you left off - Use LatticeMind locally or in the cloud with  qBraid