Shuimu Computational Materials Services

MLIP / DFT / MD simulation for advanced materials R&D

Hainan Shuimu New Materials Co., Ltd.

14+ SCI publications | DPA-4 / DPA-3.2 native | MLIP + DFT dual evidence

www: request via xinchen50@126.com

About us

We are a computational materials team with a peer-reviewed publication record in machine-learned interatomic potentials (MLIP), density functional theory (DFT) and molecular dynamics (MD). We help research groups and industrial R&D teams accelerate corrosion, catalysis, battery and coating development. Every project is delivered with raw data, publication-quality figures and a full methodology report, cross-checked with DFT where applicable.

Service catalogue

1. MLIP Training & Fine-tuning - USD 800+ / project

Train or fine-tune DPA-4 / DPA-3.2 potentials on your target chemistry. Scope: dataset preparation (DFT -> DeePMD format), training with modern schedulers, validation (energy/force MAE, MD stability). Deliverable: model file (.pt / frozen), training report, evaluation figures. Proprietary datasets stay yours.

2. High-throughput Adsorption Screening - USD 300+ / batch

Binding / adsorption energy screening of molecules on metal surfaces (fcc / bcc, (100)/(110)/(111)). 50-300 systems per batch, ranked, with literature anchoring. Deliverable: ranked table, key structures, analysis report. Ideal for catalyst and corrosion inhibitor screening.

3. Molecular Dynamics - USD 400+ / system

NVT / NVE simulations (300-400 K) of adsorbate stability, diffusion and interface behaviour. Deliverable: trajectory statistics, energy analysis, stability ranking, figures.

4. DFT Validation (CP2K) - USD 250+ / structure

Density functional theory single points, geometry optimisation and adsorption energy validation to cross-check MLIP predictions - the dual-evidence standard.

5. Full Publication Package - USD 1,200+ / project

End-to-end support: calculations, figures, tables and methodology text ready for peer-reviewed journal submission. Ideal for groups needing computational support for their manuscripts.

6. Technical Consulting - USD 80 / hour

Guidance on MLIP workflows, dataset preparation, DPA deployment on your cluster, or review of your simulation strategy.

How it works

Step 1 - Quote

Send your system details (structures, target properties, deadline). Fixed quote within 24 h.

Step 2 - Compute

50% deposit starts the project. GPU-accelerated compute with input validation and QC checkpoints.

Step 3 - QC & Deliver

Three-gate quality control: energy magnitude, element consistency, requirement match.

Step 4 - Revise

Two rounds of free revisions. Final payment on delivery. NDA / IP protection available.

Quality assurance

1) Three-gate QC: energy magnitude sanity, element composition consistency, and requirement match - applied to every deliverable. 2) Dual evidence: MLIP screening cross-checked with DFT (CP2K) where possible. 3) Publication-grade output: our own 14+ SCI record means results are formatted to journal standards by default. 4) Data security: NDA by default, dedicated compute instances, no cross-client reuse.

Pricing summary

MLIP training / fine-tuning	USD 800 - 1,500
Adsorption screening (50-300 systems)	USD 300 - 800
Molecular dynamics (per system)	USD 400 - 700
DFT validation (per structure)	USD 250 - 500
Full publication package	USD 1,200 - 2,500
Consulting	USD 80 / hour
Rush delivery	+50%

Frequently asked questions

Q: Turnaround?

A: 3-7 working days depending on scope; rush (+50%) available.

Q: What do you need from me?

A: Structure files (CIF/XYZ/POSCAR), target surface/facet, properties. We can also build structures.

Q: Payment?

A: Bank transfer or Payoneer/Wise. 50% deposit, 50% on delivery. English/Chinese invoices.

Q: Dissatisfied?

A: Two rounds of free revisions; failed calculations re-run free or refunded.

Q: Confidentiality?

A: NDA by default, dedicated instances, no cross-client data reuse.

Q: Scope you do NOT take?

A: We sell methods, tools, data and compute - not ready-made product formulations or recipe optimisation.

Q: Academic collaboration?

A: Welcome - co-authorship and collaboration agreements possible.

Q: Proprietary training data?

A: Yes - train on your data, dataset stays yours.

Get a quote within 24 hours

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