

Company Name: Rhinovate (Hong Kong) Technology Co., Limited

Position: AI for Science Algorithm Engineer

Posting Date: 5 Aug 2026

Job Description:

A. Company Profile

The company focuses on the AI for Materials / AI for Science track. Differentiated from traditional materials R&D enterprises and general large model companies, we build an integrated platform featuring "AI molecular design + computational chemistry + material simulation + automated experiments + closed-loop chemical data". Leveraging proprietary technologies to deliver projects for industrial clients, we are assembling an early core technical talent team. Through AI, scientific computing, physical experiments and data-driven methodologies, we help industrial clients accelerate new material design, property prediction, experimental verification and commercial delivery.

B. Job Responsibilities

1. Develop end-to-end AI for Science algorithms tailored to new material R&D scenarios, covering core modules including inverse generation of molecules and materials, property prediction of materials and molecules, and high-throughput material data mining.
2. Conduct scientific simulation calculations such as first-principles DFT, molecular dynamics (MD) and AIMD; build multi-scale material simulation systems by integrating machine learning potential models including MACE, DeepMD and GNN.
3. Develop scientific computing pipelines, data modeling frameworks and automated research workflows based on Python; build toolchains for AI Agents and all-in-one material computing platforms.
4. Establish a closed R&D loop of "AI prediction – computational modeling – automated experiments – data feedback – model iteration". Collaborate with industrial clients to address real-world new material R&D demands and deliver deployable algorithm solutions.
5. Collaborate cross-functionally with materials, chemistry, experimental and data teams to resolve practical technical challenges in industrial new material R&D, and participate in the full-cycle development and iteration of products from scratch.

Requirements:

A. Academic Background

Bachelor's degree or above in science and engineering disciplines including Materials Science, Chemistry, Computational Chemistry, Condensed Matter Physics, Artificial

Intelligence, Computer Science, Applied Mathematics, with solid foundational theoretical knowledge in science and engineering.

B. Technical Competencies (Partial proficiency acceptable; full mastery not mandatory)

1. Master basic theories and practical operations of first-principles and molecular simulations including DFT, MD and AIMD.
2. Familiar with Scientific Machine Learning; possess knowledge of molecular and material ML models such as GNN, MACE and DeepMD.
3. Proficient in Python development, scientific computing and data modeling; capable of independent algorithm coding and implementation.
4. Prior research or project experience in molecular generation, inverse material design, high-throughput computing or materials informatics is preferred.
5. Hands-on experience in automated research workflows, AI Agent development or scientific computing platform tool development is a plus.

C. Soft Skills & Personal Qualities

1. Strong passion for the integration of AI and new materials, AI for Science, scientific computing and material simulation.
2. Not limited to purely theoretical academic research; willing to translate technical solutions into real industrial applications.
3. Excellent self-directed learning ability and cross-disciplinary communication & collaboration skills.
4. Align with the development model of an early-stage startup; ready to deeply participate in the ground-up development of the company's core technologies.

D. Core Benefits of the Position

1. Niche High-Growth Track: A cutting-edge track leveraging AI to reshape the paradigm of new material R&D, tackling genuine pain points in industrial material development.
2. Full-Stack Technical Closed Loop: R&D led by scientists, covering the entire pipeline of AI algorithms, computational simulation, automated experiments and data iteration for comprehensive career growth.
3. Core Early-Stage Headcount: Founding team position with full involvement in the overall construction and iteration of the platform product.
4. Application-Oriented R&D: All algorithm R&D is driven by real industrial client projects, with directly commercializable research outputs.
5. Competitive Compensation Package: Highly competitive base salary plus long-term equity and stock option incentives.

Application method:

Please send resume to zhangshuang@rhinovate.tech