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Computational Chemistry Software Engineer

Apply

 Woburn, MA

At SES AI, base pay is one part of our total compensation package and is determined within a range. The base pay range for this role is between \$150,000 and \$250,000. SES AI considers several factors when extending an offer, including but not limited to, the role, function and associated responsibilities, a candidate's work experience, location, education/training, and skills.

What We Offer

- Company paid Health and Dental insurance (ability to add dependents)
- Global travel insurance for employees traveling while on business
- Company sponsored retirement plan with 100% vesting and up to 5% match.
- Life and AD&D Insurance
- Employee Assistance Program
- Six Paid Holidays, and one floating holiday per a quarter equivalent to 4 per calendar year
- 10 accrued vacation days per calendar year that increases with tenure.
- Bonus + Equity, based on position and eligibility requirements

Note: SES AI benefit, compensation, and employee stock programs are subject to eligibility requirements and other terms of the applicable plan or program.

About SES AI:

SES AI Corp. (NYSE: SES) is powering the future of global electric transportation on land and in the air with the world's most advanced Li-Metal batteries. SES AI is the first battery company in the world to accelerate its pace of innovation by utilizing superintelligent AI across the spectrum of its business, from research and development; materials sourcing; cell design; engineering and manufacturing; to battery health and safety monitoring. Founded in 2012, SES AI is an Li-Metal battery developer and manufacturer headquartered in Boston with operations in Singapore, Shanghai, and Seoul.

Learn more at [SES.AI](https://www.ses.ai)

About the Role:

The SES AI Prometheus team (AI Research) is seeking versatile Computational Chemistry Software Engineers to enhance our computational and machine learning simulation workflows. This role involves developing, optimizing, and deploying molecular simulation packages and ML models across high-performance computing (HPC) and cloud environments. You'll work in close partnership with materials scientists to streamline density functional theory (DFT) calculations, molecular dynamic (MD) simulations, manage complex orchestration tasks, and ensure reproducibility and scalability of our software solutions.

This is a remote position.

Key Responsibilities:

- **Code Development and Optimization:** Develop, optimize, and maintain custom scripts or computational packages (e.g., in Python, Fortran, C++) to streamline molecular simulations and deploy AI models effectively. Identify and resolve computational bottlenecks for faster and more accurate simulations.
- **Software Deployment:** Design and implement optimized workflows for the deployment of molecular simulation packages across high-performance computing (HPC) environments and cloud platforms. Ensure scalability and reliability of developed packages.
- **Cross-functional Collaboration:** Partner closely with scientists, engineers, and AI specialists, contributing to interdisciplinary projects and translating research requirements into efficient computational solutions.
- **Documentation and Reproducibility:** Maintain rigorous documentation standards for code, models, and deployment workflows, ensuring reproducibility and compliance with industry standards.
- **Mentorship and Documentation:** Mentor scientists on best practices in software engineering, maintain rigorous documentation for code and deployment workflows, and uphold industry standards for reproducibility and compliance.

Qualifications:

- **Experiences:** +3 years of computational chemistry software developer/engineer experiences
- **Educational Background:** Ph.D. or M.S. in Computer Science, Computational Chemistry, Chemical Engineering, Materials Science, or a related field, with a focus on molecular simulations.
- **Technical Skills:**



- Proficiency in molecular dynamics packages (e.g., LAMMPS, GROMACS, CP2K, NAMD).
- Advanced programming skills in Python, Fortran, and C++, with expertise in software development and test-driven practices.
- Familiarity with GPU-accelerated DFT packages like GPU4PySCF and machine learning frameworks for molecular property prediction.
- Experience with software package deployment, optimization, and maintenance in HPC and cloud platforms.
- Knowledge of data analysis and visualization tools (e.g., NumPy, Pandas, Matplotlib), and skills in parallel computing, multi-threading, and optimizing software for performance on large datasets.
- **Domain Knowledge:** Solid understanding of chemical interactions, thermodynamics, and statistical mechanics in molecular simulations.
- **Soft Skills:** Strong communication skills, the ability to collaborate across disciplines, and a proactive, solution-oriented approach.

Preferred Experience:

- Experience with molecular modeling tools such as Gaussian, VASP, or Quantum ESPRESSO.
- Proven track record in managing and scaling computational simulations on distributed systems or clusters.
- Familiarity with machine learning frameworks and the integration of AI for molecular property prediction.

Who Will Thrive in This Role:

- A skilled developer passionate about molecular simulations and machine learning, with a commitment to creating efficient, scalable, and robust software solutions.
- An effective problem solver who values documentation and reproducibility.
- A proactive mentor and collaborator who can translate complex research needs into practical computational tools.

Apply for this job

* indicates a required field

First Name *

Last Name *

Email *

Phone

Resume/CV

Attach

Dropbox

Google Drive

Enter manually

Accepted file types: pdf, doc, docx, txt, rtf

Cover Letter

Attach

Dropbox

Google Drive

Enter manually

Accepted file types: pdf, doc, docx, txt, rtf

LinkedIn Profile

Website



Voluntary Self-Identification

For government reporting purposes, we ask candidates to respond to the below self-identification survey. Completion of the form is entirely voluntary. Whatever your decision, it will not be considered in the hiring process or thereafter. Any information that you do provide will be recorded and maintained in a confidential file.

As set forth in SES's Equal Employment Opportunity policy, we do not discriminate on the basis of any protected group status under any applicable law.

Gender

Select...



Are you Hispanic/Latino?

Select...



[Race & Ethnicity Definitions](#)

If you believe you belong to any of the categories of protected veterans listed below, please indicate by making the appropriate selection. As a government contractor subject to the Vietnam Era Veterans Readjustment Assistance Act (VEVRAA), we request this information in order to measure the effectiveness of the outreach and positive recruitment efforts we undertake pursuant to VEVRAA. Classification of protected categories is as follows:

A "disabled veteran" is one of the following: a veteran of the U.S. military, ground, naval or air service who is entitled to compensation (or who but for the receipt of military retired pay would be entitled to compensation) under laws administered by the Secretary of Veterans Affairs; or a person who was discharged or released from active duty because of a service-connected disability.

A "recently separated veteran" means any veteran during the three-year period beginning on the date of such veteran's discharge or release from active duty in the U.S. military, ground, naval, or air service.

An "active duty wartime or campaign badge veteran" means a veteran who served on active duty in the U.S. military, ground, naval or air service during a war, or in a campaign or expedition for which a campaign badge has been authorized under the laws administered by the Department of Defense.

An "Armed forces service medal veteran" means a veteran who, while serving on active duty in the U.S. military, ground, naval or air service, participated in a United States military operation for which an Armed Forces service medal was awarded pursuant to Executive Order 12985.

Veteran Status

Select... ▼

Voluntary Self-Identification of Disability

Form CC-305

OMB Control Number 1250-0005

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Expires 04/30/2026


Why are you being asked to complete this form?

We are a federal contractor or subcontractor. The law requires us to provide equal employment opportunity to qualified people with disabilities. We have a goal of having at least 7% of our workers as people with disabilities. The law says we must measure our progress towards this goal. To do this, we must ask applicants and employees if they have a disability or have ever had one. People can become disabled, so we need to ask this question at least every five years.

Completing this form is voluntary, and we hope that you will choose to do so. Your answer is confidential. No one who makes hiring decisions will see it. Your decision to complete the form and your answer will not harm you in any way. If you want to learn more about the law or this form, visit the U.S. Department of Labor's Office of Federal Contract Compliance Programs (OFCCP) website at www.dol.gov/ofccp.

How do you know if you have a disability?

A disability is a condition that substantially limits one or more of your "major life activities." If you have or have ever had such a condition, you are a person with a disability. **Disabilities include, but are not limited to:**

- Alcohol or other substance use disorder (not currently using drugs illegally)
 - Autoimmune disorder, for example, lupus, fibromyalgia, rheumatoid arthritis, HIV/AIDS
 - Blind or low vision
 - Cancer (past or present)
 - Cardiovascular or heart disease
 - Celiac disease
 - Cerebral palsy
- 

- Deaf or serious difficulty hearing
- Diabetes
- Disfigurement, for example, disfigurement caused by burns, wounds, accidents, or congenital disorders
- Epilepsy or other seizure disorder
- Gastrointestinal disorders, for example, Crohn's Disease, irritable bowel syndrome
- Intellectual or developmental disability
- Mental health conditions, for example, depression, bipolar disorder, anxiety disorder, schizophrenia, PTSD
- Missing limbs or partially missing limbs
- Mobility impairment, benefiting from the use of a wheelchair, scooter, walker, leg brace(s) and/or other supports
- Nervous system condition, for example, migraine headaches, Parkinson's disease, multiple sclerosis (MS)
- Neurodivergence, for example, attention-deficit/hyperactivity disorder (ADHD), autism spectrum disorder, dyslexia, dyspraxia, other learning disabilities
- Partial or complete paralysis (any cause)
- Pulmonary or respiratory conditions, for example, tuberculosis, asthma, emphysema
- Short stature (dwarfism)
- Traumatic brain injury

Disability Status

Select... ▼

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