Department of Chemical, Biological, and Materials Engineering
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URL: Simmons Research Group

Dear SES AI Corp. Hiring Committee, April 7, 2025

I am writing to express my enthusiastic interest in the **Computational Chemistry Software Engineer position** at SES AI. With over a decade of experience designing scalable molecular simulation frameworks and mentoring interdisciplinary research teams, I am excited by SES AI's mission to integrate AI into battery innovation – a goal that aligns deeply with both my expertise and long-term aspirations.

My favorite aspect of my career has been the challenge of optimizing simulation and workflow code to enable high-throughput scientific discovery while maintaining rigorous physical accuracy. In both my postdoctoral and doctoral work, I've architected custom C++/CUDA and Python-based tools for molecular modeling, with an emphasis on iterative performance tuning, bottleneck resolution, and robust documentation. Whether designing GPU-accelerated Monte Carlo engines from scratch or managing SLURM-based job arrays to process over 50 TB of simulation data, I bring a mindset that blends scientific rigor with engineering scalability.

Equally rewarding has been my role as a mentor. I've guided 15+ researchers across multiple institutions and academic backgrounds, equipping them with not only technical tools like Git and HPC scripting, but also sustainable habits for documentation, debugging, and problem-solving. Watching them grow into confident, impactful scientists has been one of the most meaningful parts of my journey.

Technically, I bring breadth and depth across molecular dynamics (LAMMPS, GROMACS), Monte Carlo methods, statistical mechanics, free energy simulations, and experimental validation – applied across polymers, nanoparticles, and composite materials. My work has consistently focused on answering physics-based questions using tailored, accurate, and scalable simulations. Looking ahead, I am eager to further integrate AI methodologies into these frameworks to accelerate insight generation and model evolution – especially in dynamic systems like energy materials.

I would be thrilled to bring this combination of simulation expertise, collaborative spirit, and continuous improvement mindset to the Prometheus team at SES AI. Thank you for considering

my application. I look forward to the opportunity to contribute to your innovative work.

Kind regards,

Pierre Kawak, Ph.D.
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