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Applied Research Scientist, Molecular Simulation

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Company: InstaDeep Location: London Area Category: other-general

InstaDeep is looking for an Applied Research Scientist to join our expanding team. Applied Research Scientists at InstaDeep develop algorithms and data pipelines focused mainly, but not exclusively, on physics-based methods. As part of the BioAI team, you will be contributing to the development of new approaches in molecular modelling, protein interactions, protein design and other related domains by applying your technical, analytical, and research skills. You will understand the underlying biology and engineering problems and follow the latest developments in machine learning and classical modelling algorithms to identify and harness the right technologies to solve the problems, improve the existing solutions and deploy them. You will collaborate with a multi-functional team, experiment with different approaches, analyse and communicate the results in order to deliver proof of concepts and ensure continuous improvement and maintenance for industrialised solutions.Keywords: Computational molecular Physics, Structural Biology, Computational Chemistry, Protein Interactions, Protein Design, Molecular Dynamics, Monte Carlo, Enhanced Sampling, Machine Learning, Deep Learning, Statistics, Data ScienceResponsibilitiesDesign, implement and deliver complex pieces of research in the area of computational molecular physics/biology.Implement and test pioneering enhanced sampling methods and free energy calculation techniques that leverage and supplement machine learning approaches.Communicate and collaborate with research engineers in a multi-functional team to integrate simulation-based solutions into drug discovery platforms and ensure they are robust, maintainable and easily used by scientistsReport results clearly and efficiently, both internally and externally, verbally and in writing. Understand and follow the latest

biology/biophysics and machine learning developments for relevant applications.Write maintainable and modular code together with concise documentation. Required SkillsMaster, PhD degree or equivalent experience in Biophysics, Chemistry, Biochemistry, Computational Chemistry/Biology or any related scientific field. A proven track record of methods development/deployment for molecular simulations and/or Computational Chemistry/BiologyGood software engineering experience (Python, Docker, Linux, Git).Experience with protein structure modelling and/or simulation.Excellent communication skills in English.Appropriate work permit for the considered location.Nice to haveExperience with quantum mechanics software and methods. Experience running jobs on cloud-based infrastructure at scaleFamiliarity with in-silico drug discovery pipelinesA real passion for delivering computational solutions for complex biological problemsBenefitsCompetitive compensation package. Working in small, diverse teams where you can make an impact.Varied challenges across industries.Cooperation across European, US, and African offices.Annual offsite events.Our commitment to our peopleWe empower individuals to celebrate their uniqueness here at InstaDeep. Our team comes from all walks of life, and we're proud to continue encouraging and supporting applicants from underrepresented groups across the globe. Our commitment to creating an authentic environment comes from our ability to learn and grow from our diversity, and how better to experience this than by joining our team? We operate on a hybrid work model with guidance to work at the office at least 2 to 3 days per week to encourage close collaboration and innovation. We are continuing to review the situation with the well-being of InstaDeepers at the forefront of our minds. Right to work: Please note that you will require the legal right to work in the location you are applying for.

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