Machine Learning/Computational Chemist
Cambridge, MA

Kebotix is a technology company leading the materials industry towards the age of high-speed innovation using artificial intelligence and robotic automation. Our technology is centered around smart algorithms that allow for discoveries of new materials that solve the problems around us.

We are looking for a Machine Learning/Computational Chemist who will be a member of a multi-disciplinary customer-centric project team working in a fast-paced startup environment. You will be responsible for developing and applying state-of-the-art deep learning and computational chemistry tools for design of novel chemicals and materials. Further, you will work on integrating the machine learning tools into the data and workflow pipelines embedded in a larger discovery platform for the design of functional materials, green chemistry, and pharmaceuticals. Depending on your level of seniority, you will take an active role in project management, ensuring successful project execution.

Qualifications and Experience

- Ph.D. or equivalent in Chemistry, Biology, Materials Science, Physics, or a related field
- Experience in computational chemistry, organic chemistry, and/or physical chemistry
- Experience with cheminformatics and related libraries (e.g., RDKit)
- Experience with computational chemistry methods (e.g., ab-initio, DFT, MD, Semi-empirics, DFTB, xTB) for prediction of properties and reactivity of small molecules, oligomers and polymers.
- Experience with state-of-the-art machine learning methods such as Graph Convolutional Networks, Transformer architecture, and probabilistic modeling is a plus
- Experience with generative models is a plus (e.g., VAE, GAN, Flow)
- Experience with Monte-Carlo tree search, genetic algorithms, and reinforcement learning is a plus
- Experience with deep learning frameworks (e.g., PyTorch, Tensorflow)
- Proven track record of publications in scientific journals in the chemistry, physics, or computer science communities
- Hands-on experience in programming, e.g., Python
- Excellent oral and written communication, presentation, and analytical skills

Please apply directly on our website www.kebotix.com/careers

We offer an excellent career opportunity and an exciting working environment. With an entrepreneurial spirit and a dynamic friendly environment, we strive to ensure that the success of our company brings both professional and financial rewards to all of our employees. We look forward to receiving your application!

Kebotix is an Equal Opportunity Employer committed to no discrimination because of race, color, creed, marital status, age, religion, sex, national origin, citizenship, sexual orientation, gender identity or expression, genetic information, disability, protected veteran, or any other legally protected characteristic.