



Powering molecular discovery through quantum algorithms and machine learning

Machine Learning or Cheminformatics Scientist - Position Available

Position

Entos Inc. provides tools for molecular and materials discovery through the use of physics-based machine learning. We seek a Machine Learning or Cheminformatics Scientist to advance our core mission of accelerating molecular discovery through deep-learning and quantum mechanics.

Responsibilities

- Work with a cross-disciplinary team of scientists and engineers to develop and deploy models for prediction of molecular properties
- Develop and maintain pipelines for data collection and cleaning, machine learning featurization and training, and model validation
- Develop novel feature extraction strategies and model architectures
- Implement and benchmark existing state-of-the-art models

Preferred Qualifications

- Postgraduate and/or industry experience in property prediction for applications in chemistry/materials/biology, including cheminformatics and ADME-Tox
- Programming expertise, inc. Python and the PyData stack (numpy, pandas, scikit-learn, etc.)
- Experience with traditional (e.g. tree-based) and/or deep learning methods
- Experience in graph neural networks and/or generative models
- Experience with cheminformatics tools, such as RDKit

Also

- Competitive compensation, inc. equity, benefits (medical, dental, vision), and 401K matching
- Location in Pasadena, CA is preferred

Company Background

Entos was founded in 2019 by faculty from Caltech and the University of Bristol and is situated at the interface of quantum chemistry, machine learning, and drug discovery. We seek to bring quantum simulation to real-world problems, with the aim of disrupting entire industries. Our team is tight-knit and rapidly growing. We are committed to building an inclusive work environment at Entos, where a diverse group of talented people work together to create awesome technologies. If you have the curiosity, passion, and collaborative spirit, join us and let's change the world together!

Submit a Cover Letter and Resume to: Jeanne Grover, jeanne@entos.ai