Job Title: Cheminformatics Group Leader

Location: Santa Fe, New Mexico

Education: Master or PhD in Computation Chemistry, Computer Science or closely related fields

Experience: 5+ years of experience using Python &/or C++ for science development

Travel: Occasional

Manage Others: Yes

Job Description:

OpenEye Scientific Software, Inc. seeks to hire a professional software developer to lead a team delivering scientific solutions to drug discovery problems.

The successful candidate’s team will have shared responsibility for delivering established products, building new technologies into customer solutions, and establishing new algorithms for cheminformatics and machine learning in drug discovery. You will be able to deploy your solutions on Orion, the most exciting cloud platform available today for drug discovery.

The team you will join includes several PhD level scientific developers with expertise in small molecule and protein computational chemistry and long track records of delivering C++ applications and core software libraries to solve drug discovery problems.

We hope you will bring your expertise in cheminformatics and machine learning to our group. We expect your primary contribution will be to develop ML models for drug discovery. You will be delivering both your new models and tools for customers to build their own models in Orion, OpenEye’s cloud platform. In addition, you will take on a role in the life of learning, maintaining and developing the full range of OpenEye cheminformatics tools.

This position is available at our headquarters in Santa Fe, NM. Relocation assistance will be provided.
What we do:

- Write state-of-the-art scientific software tools for drug discovery
- Perform molecule similarity search and substructure search on hundreds of millions of molecules in seconds
- Calculate, analyze and visualize complex chemical information
- Name chemical compound and calculate molecular properties
- Help customers solve problems

What we use:

- Python, C++, Java, C#
- cmake, swig, git, Jupyter, conda, pip, Atlassian tools: JIRA, bitbucket, Fisheye
- Multi-platform development environment
- Orion: A cloud-platform for high-performance scientific computing

Requirements:

What you bring:

- Leadership skills including social skills, communication skills, ability to plan and schedule, ability to outline a scientific vision, and the ability to inspire and encourage colleagues
- Master or PhD in Computational Chemistry, Computer Science or closely related fields
- Desire to learn new ideas and technologies
- 5+ years of experience using Python and/or C++ for scientific development
- A strong ability to give scientific talks covering your own and your colleague's work
- Knowledge of the cheminformatics and drug discovery literature
- Thorough understanding of professional software development practices & tools
- Familiarity with several of the scientific python tools such as Jupyter, NumPy, SciPy, Pandas, Matplotlib, ScikitLearn, Tensor Flow and PyTorch

What we prefer

- Leadership experience
• Teamwork
• Attention to detail
• Excellent communication skills
• Scientific and technical innovation
• Experience designing new scientific APIs
• Knowledge of building, evaluating and improving scientific models, including shallow and deep learning techniques.
• The ability to write new code when necessary, use old code when appropriate
• Expert knowledge of OEChem, RDKit or closely related cheminformatics platforms
• Experience with scientific pipelining tools such as Pipeline Pilot or Knime
• Ability to work under a development schedule, balancing features and delivery deadlines

Application Contact Information:

To apply please Email cover letter and resume along with code sample or/and github account to: hr@eyesopen.com