



THE UNIVERSITY  
*of* EDINBURGH

## **‘Supporting the OpenMM Community-led Development of Next-Generation Condensed Matter Modelling Software’**

3-year research software engineer position, Salary: £34,304 - £40,927 (UE07)

Line manager: Dr Julien Michel, School of Chemistry School of Chemistry, University of Edinburgh

An exciting position is available for a research software engineer for 36 months. The RSE will be supervised by Dr. Julien Michel (JM) and based in the School of Chemistry at the University of Edinburgh. The RSE will play a leading role in the delivery of the EPSRC-funded Software for Research Communities project: “Supporting the OpenMM Community-led Development of Next-Generation Condensed Matter Modelling Software”. The RSE will be co-supervised by Dr Daniel Cole (Newcastle University), Prof Fernanda Duarte (University of Oxford), Dr Tobias Grosser (Edinburgh University).

The RSE will work primarily on the implementation of state-of-the-art machine learning-based (ML) potentials in the OpenMM atomistic software library ([www.openmm.org](http://www.openmm.org)). The work will be carried out in close collaboration with an international consortium of OpenMM developers in the US and the EU to deliver to the community a library of extensible Machine Learning (ML) potentials that can be efficiently deployed on current GPUs and emerging AI-hardware accelerators. The RSE will develop standardised interfaces to integrate OpenMM software with other popular software used by the biomolecular simulation community. The RSE will coordinate with domain experts in molecular simulations to assemble production hybrid MD/ML pipelines for scientific use cases. A significant focus of the RSE will be provision and delivery of training support to the growing community of users of OpenMM in the UK and beyond.

More details about the project are available here:

<https://gow.epsrc.ukri.org/NGBOVViewGrant.aspx?GrantRef=EP/W030276/1>

There is some flexibility with the starting date, but the post-holder is expected to be in position by November 1<sup>st</sup> 2022 at the latest.

Applications will be considered as they are received. Applicants are strongly encouraged to contact Dr Julien Michel ([julien.michel@ed.ac.uk](mailto:julien.michel@ed.ac.uk)) for informal inquiries about the position before submitting a formal application.