

Title: Engineer – Atomistic Simulation R&D
Report to: Chief Scientific Officer (CSO) and Chief Technology Officer (CTO)
Salary: £35k- 42k plus benefits
Job type: Full time, Permanent

# Job description:

Under the direction of the CSO and CTO of the company, the Simulation Engineer is responsible for modelling the electronic and magnetic structure of novel materials and corresponding transport properties of nano-scale multilayer systems; designing novel memory devices based on physical properties of the constituent materials; computational screening of families of materials to optimize the performance of individual devices and final products; analyzing large volumes of numerical data, reporting results, and formulating strategies for refined material searches; conducting root cause analysis and implementing corrective action; developing and implementing procedures for transitioning new products into the production line; reviewing, updating, and maintaining documentation and process instructions. This position is located in London, UK.

# Key responsibilities:

- Develop atomistic/quantum models of multi-ferroic tunnel junctions
- Apply density functional theory (DFT) to simulate ground-state electronic and magnetic structure of novel materials and multilayers
- Apply non-equilibrium Green's function method (NEGF) or Landauer-Buttiker method to obtain transport properties of a tunnel junction
- Analyse numerical data and formulate strategies for further simulations or experimental verification
- Perform Technology Computer Aided Design (TCAD) simulations to resolve memory device issues
- Collaborate closely with experimental teams; Use experimental feedback to refine the material screening and device design
- Identify and implement best practices for quality and efficiency
- Run parallelized numerical simulations efficiently using commercially available software on a Linux computer system
- Cooperate with support personnel in order to optimise the usage of the available hardware
- Conduct root cause analysis and implements corrective action if required
- Respond to inquiries from other team members, managers, or departments
- Adhere to all safety policies and procedures as required



## Job requirements

Minimum qualifications

- Phd in Materials Science, or Solid-State Physics, and/or equivalent relevant experience;
- Minimum 5 years of hands-on experience with DFT electronic structure simulations
- Experience with transport simulations, preferably based on NEGF
- Relevant track record in simulating tunnelling magneto resistance (TMR) or magnetic properties of thin films and multilayers
- Strong knowledge and experience in analysing extensive numerical data, preferably using scripting
- Proficient use of Microsoft Office

Knowledge, Skills, and Abilities:

- Working knowledge of DFT and its applications to magnetic solid-state systems at the nano-scale; previous experience with Vienna Ab-initio Simulation Package (VASP) is preferred
- Working knowledge of methods to compute transport properties of tunnel junctions; previous experiences with Quantum ATK (Synopsys, Inc.) or Smeagol (<u>www.smeagol.tcd.ie</u>) and or Siesta are a plus.
- Familiarity with the Unix/Linux environment and the command line
- Ability to run numerical simulations on a multicore computer with a job scheduling software (PBS – Torque)
- Ability to develop one's own scripts in Python to post-process the output of DFT and transport simulations (e.g., with the help of libraries such as Numpy, Scipy, Matplotlib)
- Ability to draw conclusions based on the computed data and to provide guidance for experimental colleagues
- Ability to incorporate feedback from experiments into a subsequent round of simulations and material screening
- Knowledge and ability to use Microsoft Office applications to create spreadsheets, Word documents, and presentations
- Ability to communicate effectively, both verbally and in writing, with all levels of contractors, consultants, employees, and management
- Ability to work productively and collaboratively with all levels of employees and management
- Ability to comply with all safety policies and procedures
- Demonstrated organizational and time management skills
- Demonstrated problem-solving and trouble shooting skills
- Flexible and able to prioritize



# **Working Conditions**

Simulation Engineer works primarily in an office environment from Monday to Friday. The schedule may be altered from time-to-time to meet business or operational needs; may travel from building-to-building and travel to different cities or globally as needed. The simulation engineer operates a computer and enters information using a keyboard, operates a telephone, and other office equipment.

# **Company:**

LoMaRe Technologies is a new semiconductor start-up developing emerging non-volatile memory (NVM) technologies with proprietary intellectual property.

Headquartered in London, UK, LoMaRe is a spin-off company from world leading institution Imperial College London. Our company's ambition is to commercialise scientific innovation and we are looking to add experienced experts to join our team in London to develop memory technologies. Apply to become a part of a future leader in semiconductor chip technology and join a dynamic fast-paced and friendly working environment with an ambitious and success-focused team.

To apply, please send CV to Dr. Andrei Mihai, jobs@lomaretech.com.

