

Job opening: Marie Curie PhD fellowship – Theoretical Physics / Chemistry – Machine Learning / Software Development

Summary

SCM, a scientific software company located in Amsterdam, is looking for a **PhD student** who will research and implement new **machine learning (ML) methods** for calculating accurate **infrared/Raman/UV-VIS/X-ray spectra** of molecules and materials.

The work will build upon and improve SCM's existing methods for theoretical spectroscopy, which include density functional theory, density functional-based tight binding, and GW. The focus of the project lies in the **development of methods and software** to help researchers around the world predict more accurate spectra.

The position is part of the European Commission-funded **Doctoral Network EUSpecLab**, a collaboration between several universities and companies. Salary conditions, travel/mobility allowances, and benefits will follow the attractive EU amounts for Researchers in the [HORIZON-MSCA-2021-DN-01](#) call.

The position is open to

- ML MSc graduates with an interest in chemistry/physics, and
- theoretical chemistry/physics MSc graduates with an interest in ML.

We hope that the new candidate can join us as soon as possible, with **1 September 2022** as the earliest possibility. For an excellent candidate a later start date can be discussed.

EUSpecLab, supervision and training

The EUSpecLab project contains a mix of 11 theoretical research-oriented PhD projects. The candidate will be enrolled in a PhD program at the Vrije Universiteit Amsterdam where Prof. Lucas Visscher will act as PhD supervisor, with experienced scientists at SCM, including Dr. van Lenthe and Dr. Egidi (DFT methods for spectroscopy) and Dr. Hellström, Dr. Spiering and Dr. Austin (Machine-learning and related mathematical techniques) as co-supervisors.

Planned research visits to academic collaborators:

- Prof. Patrick Rinke's group in Aalto, Finland: 3 months
- Prof. Silvana Botti's group in Jena, Germany: 3 months

- Research actions are organized in conjunction with local and network-wide training, including academic and industrial specialist courses, transferable skills training, (international) workshops and training-through-research. The training events are dispersed throughout the timeline of the project, providing an ideal platform for the Researchers to flourish and become future leaders in academic or industrial research

Job requirements

Requirements:

- **The key point:** proven algorithm and software development skills, combined with a thorough knowledge of either theoretical spectroscopy, density functional theory, or machine-learning methods.
- Being able to quickly grasp complex mathematical ideas in scientific publications, improve upon them, and convert them into clean and efficient source code.
- MSc degree in Theoretical Physics/Chemistry or Machine Learning.
- Not being in possession of a PhD degree.
- Good written and verbal communication skills in the English language.
- Willingness to relocate between Amsterdam, Aalto, and Jena, with associated costs covered by the project.

Desirable additional knowledge and experience:

- ML best practices, uncertainty quantification
- Δ -ML, optimal transport, applied ML experience for chemistry or physics
- IR/Raman/UV-VIS/X-ray spectroscopy
- Density functional theory, linear response theory, quantum mechanics, molecular symmetry
- Some experience with programming in a team, in a large-scale software package (>100,000 lines of code).
- Working knowledge of Fortran(90) and Python
- General programming skills (UNIX, debugging, etc.).
- Team player, with good two-way communication skills, highly self-motivated and able to work independently with excellent time management skills.

What we offer

The PhD fellowships will consist of an initial 3-year full-time position, with a possible extension. The start date would be as soon as possible after 1 September. Salary and secondary benefits will follow EU rules for salaries of Doctoral Network Researchers:

- Supergross monthly living allowance: 3726.40 Euro / month, which includes the 9.6% extra due to the country correction coefficient of 109.6% for The Netherlands for the entire period.
- Additional monthly mobility allowance of 600 Euro / month.

- Additional monthly family allowance of 660 Euro / month for researchers who have a family (regardless of whether the family will move with the researcher or not).

In addition, the EU provides funding for training and transfer of knowledge expenses to the institutes. Tax benefits (significant parts of salary and/or allowances paid tax-free) may be applicable in The Netherlands (depending on circumstances) for a successful candidate from abroad.

SCM offers 34 paid holidays per year and flexible working hours as well as occasional remote work options. Employees are enrolled in the ABP pension fund.

The Hosts

About SCM

Software for Chemistry & Materials B.V., SCM, is an independent spin-off company of the Vrije Universiteit Amsterdam, The Netherlands employing approximately 25 highly-educated people. SCM develops, maintains, and markets the **Amsterdam Modeling Suite**, used by computational (quantum) chemists, physicists and materials scientists in academia and industry. It includes the Amsterdam Density Functional (ADF) molecular DFT program, the periodic structure DFT program BAND, the reactive molecular dynamics program ReaxFF, approximate DFT (DFTB) software, Machine-Learning Potentials and Classical Force Fields and the COSMO-RS module for thermodynamics of mixed liquids, as well as their respective graphical interfaces and python scripting environments and workflows.

SCM has its office space on the VU campus, at walking distance from the Amsterdam-Zuid train station. We also extensively collaborate with many academic groups and household-name industrial partners worldwide. The working atmosphere at SCM is that of an informal team of PhDs and PhD students doing intellectually challenging work. SCM is located in the same wing of the building and closely interacts with the well-known **Theoretical Chemistry** (TC) professors at the VU: Visscher, Gori-Giorgi, Bickelhaupt and Fonseca Guerra as well as emeritus professor Baerends. The TC group consists of about 30 people, including a very international mix of PhD students, postdocs, and guests. SCM is a science-focused company which has been around for over 25 years. It is financially solid, growing, and profitable. SCM is located in Amsterdam, the very lively, enjoyable and internationally oriented (with 178 different nationalities) capital of The Netherlands. Thanks to its high quality of living and dynamism, Amsterdam has been elected as **“best city for Millennials to live”**, **4th most dynamic European city** and **best European tech city to work in**, and it consistently ranks high in Mercer’s annual Quality of Living surveys (**11th best in the world, in 2019**).

Eligibility

We especially invite women to apply. EU mobility rules apply. In principle, applicants can have any nationality and any current residence (although immigration rules apply, favoring EU applicants). Candidates who have already been awarded a PhD degree are not eligible.

Further information, applying

Detailed information on SCM and its software can be found at <https://www.scm.com/>

Those interested in this position are encouraged to contact project partners for further information:

- SCM, Dr. S.J.A. van Gisbergen, CEO: jobeuspeclab@scm.com
- Prof. L. Visscher: [l dot visscher at vu dot nl](mailto:l.visscher@vu.nl)

Job applications can only be sent by email to jobeuspeclab@scm.com. The application procedure will run until the position is filled. Applications should contain

- CV
- Data to support that you are an excellent young scientist
- Letter explaining the detailed motivation for applying
- List of publications
- Clear and complete summary of your programming and method development experience (as opposed to using standard existing software).

References may be requested at a later stage.