



## **Job opening: Marie Curie PhD fellowship Theoretical Condensed Matter Physics – Machine Learning – Software Development**

The position is part of the European Commission-funded Doctoral Network ***EUSpecLab***, a collaboration between 23 universities and companies. Salary conditions, travel/mobility allowances, and benefits follow the attractive EU amounts for Researchers in the **HORIZON-MSCA-2021-DN-01** call. The ***EUSpecLab*** project contains a mix of 11 theoretical research-oriented PhD projects.

The position is open to

- Modelling, numerical analysis MSc graduates with an interest in physics
- Theoretical chemistry/physics MSc graduates with an interest in Machine Learning
- Machine Learning MSc graduates with an interest in physics

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.

The candidate will be enrolled in a PhD program at the University of Rennes-1 (France). The supervisor will be Dr. Didier Sébilleau and the co-supervisor Prof. Ján Minár from the University of West Bohemia (Czech Republic). It will involve mandatory visits to academic and industrial collaborators:

- Dr. Heike Herper (University of Uppsala – Sweden): 1 month
- Dr. Luuk Visscher (Vrije Universiteit Amsterdam – Netherlands): 1 month
- Prof. Keisuke Hatada (University of Toyama – Japan): 2 months
- Scienta-Omicron AB (Uppsala – Sweden): 3 months
- Prof. Ján Minár (University of West Bohemia – Czech Republic) : 3 months

**PhD subject:** *Full potential spin-polarised relativistic multiple scattering photoelectron diffraction/ X-Ray absorption modelling of magnetic 2D and 3D materials*

### **Objectives:**

To develop a full potential spin-polarised photoelectron diffraction/ X-ray absorption computer (XAS) code within the existing *MsSpec* and *FPMS* computer packages. The *MsSpec* package is a spin-independent set of programs modelling different spectroscopies for atomic structure analysis. The *FPMS* package, developed by at the university of Toyama (Japan) is a full-

potential spin independent XAS code. The Researcher will incorporate spin-polarization, in order to access the magnetic structure, and also methods to allow the treatment of strongly correlated systems. More precisely:

- Spin-polarised relativistic multiple scattering module for MsSpec and FPMS
- Full potential module for MsSpec (through University of Uppsala secondment)
- Interface with state-of-the-art electronic structure codes (DFT, GW, ...), through University of Uppsala and Amsterdam secondments.
- DMFT (Dynamical Mean Field Theory) read-in or built-in to treat correlations (for low kinetic energies) (through University of West Bohemia secondment).
- Testing against experimental data provided by University of West Bohemia and Paul Scherrer Institute (CH).
- Structure optimisation using machine-learning for the comparison between calculated and experimental spectra (based on SCIENTA-OMICRON secondment for the knowledge of how experimental spectra are treated)

### **Expected Results:**

An easy-to-use open-source computer code released within the *MsSpec* package:

- A computer code that can exchange data easily with *ab initio* electronic structure codes through a common data format based on HDF5.
- A code that can extract from experimental spectra both the atomic structure and the magnetic structure, especially in the area close to the surface.
- First experimental results on the new generation of spin-polarised photoelectron diffraction set-ups.

### **Job Requirements:**

- Key point: proven algorithm and software development skills, combined with a thorough knowledge of either theoretical spectroscopy, 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, Modelling or Machine Learning
- Good written and verbal communication skills in the English language.
- Willingness to relocate between Rennes, Uppsala, Pilsen, Amsterdam and Toyama with associated costs covered by the project.

### **Desirable additional knowledge/skills:**

- Quantum mechanics, scattering theory
- Some experience with programming in a large-scale software package (> 100,000 lines of code)
- Photoemission, X-ray absorption spectroscopy
- Working knowledge of Fortran(90) and Python
- General programming skills (UNIX/Linux, debugging, version control software, etc.)
- Machine learning best practices

### **What we offer:**

The PhD fellowships will consist of a 3-year full-time position. 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:

- Gross monthly living allowance: 3957.6 € / month, which includes the country correction coefficient of 116.4% for France for the entire period.
- Additional monthly mobility allowance of 600 € / month.
- Additional monthly family allowance of 660 € / 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.

### **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. In addition, candidates who have already spent more than 12 months in France within the last 3 years are not eligible (unless as part of a procedure for obtaining refugee status under the Geneva Convention).

### **Application:**

Job applications can only be sent by email to [didier.sebilleau@univ-rennes1.fr](mailto:didier.sebilleau@univ-rennes1.fr). 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.