

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 **HORIZONMSCA-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 West Bohemia (Pilsen, Czech Republic). The supervisor will be prof. Ján Minár from the University of West Bohemia and the co-supervisor Dr. Matthias Muntwiler from the Paul Scherrer Institut (PSI, Switzerland). It will involve mandatory visits to academic and industrial collaborators:

- Patrick Rinke (Aalto University – Finland): 2 month
- Matthias Verstraete (University of Limerick – Ireland): 2 month
- Didier Sébilleau (CNRS, Rennes – France): 2 months
- Rastislav Varga (RVmagnetics, a.s., Košice, company – Slovakia): 3 months

PhD subject: *Electronic structure of lanthanide-doped materials for phosphor-converted white light emitting diodes*

Objective:

The main scientific objective of this combined theoretical and experimental work is to gain insight into the physical mechanisms that influence the efficiency and thermal quenching of materials used for phosphor-converted LEDs. We will analyse temperature dependent trends in the electronic properties and their signatures in various spectroscopies when chemical types, concentrations and geometrical arrangements of the dopants and of the ligands are varied. Therefore, the following tasks will be addressed:

- The Researcher will implement ML for displacements (provided by UL) and combine it with one-step model of photoemission.
- ML supported study of thermal quenching and its impact on the quantum efficiency of luminescent materials by alloy analogy model.
- Analyzing the results in terms of their trends with chemical composition, concentration and geometrical arrangements of dopants and ligands.
- Experimentally identify signatures and analyze ML predicted thermal quenching behavior by valence band photoemission spectroscopy of several
- lanthanide-doped silico-oxo-nitrides.

Expected Results:

- Description of the role of exchange-splitting and spin-orbit coupling for electronic transitions localized close to the lanthanide dopant.
- Understanding the role of electronic correlations and disorder in lanthanide-doped phosphors. Developing new and improving existing schemes for description of excited states of dopants, with emphasis on electron-hole interaction.
- Study of structure related properties around lanthanide impurities and the impact on the quantum efficiency of the luminescent materials. Description of thermal quenching by means of alloy analogy model and experimental identification the markers of vibrations in photoemission and XAS spectra.
- Development of the interface between ML for displacements and spectroscopic modules of the KKR package.

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 Pilsen/Czech Republic, Aalto/Finland, Limerick/Ireland, Rennes/France, Košice/Slovakia, Villigen/Switzerland 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, debugging, 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:

- Supergross monthly living allowance: **2689,40 €** / month, which includes due the country correction coefficient of 79.1% for the Czech Republic 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 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 the Czech Republic within the last 3 years are not eligible (unless as part of a procedure for obtaining refugee status under the Geneva Convention).

How to apply:

Applications as single pdf-document, including:

- Cover and motivation letter,
- Structured CV,
- Contact details of two referees,
- Academic transcripts and (link to) Master thesis,

please send to **prof. Dr. Jan Minar:** jminar@ntc.zcu.cz

Department website:

https://www.ntc.zcu.cz/en/Research/Research_topics/Advanced_Materials.html

Information about Pilsen:

<https://www.pilsen.eu/citizen/>