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

Summary

The nanomat research group, based in the Physics Department of the University of Liège (Belgium), is looking for a **PhD student** who will research and implement new **machine learning (ML) methods** for calculating **vibrational and thermal effects in infrared/Raman and X-ray spectra** of bulk and nanostructured materials.

The work will build upon cutting edge methods and tools for theoretical spectroscopy, which include density functional theory, density functional perturbation theory and the temperature dependent effective potential (TDEP) method. The focus of the project lies in the **development of methods and software** to discover novel thermal and vibrational effects in spectroscopy, and their application to catalytic materials in collaboration with Toyota Motors Europe.

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 scales for Researchers in the HORIZON-MSCA-2021-DN-01 call.

The position is open to
- ML MSc/MEng graduates with an interest in physics/chemistry/materials, and
- theoretical physics/chemistry/materials MSc/MEng graduates interested 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 exceptional candidate a later start date can be discussed. https://ec.europa.eu/programmes/horizon2020/en/h2020-section/marie-sklodowska-curie-actions

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 with the doctoral school in Physics of the University of Liege where Prof. Matthieu Verstraete will act as PhD supervisor, with active support from a close-knit team of researchers in electronic structure. http://www.nanomat.ulg.ac.be/?page_id=10.

Planned research visits to network collaborators:

- **Experimental characterization lab at** Toyota Motor Europe Zaventem, Belgium: 3 months

- Prof. Miguel Marques in the University of Halle, 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 distributed along 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 at least one of: 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.
- Excellent presentation, written and verbal communication skills in English.
- Willingness to relocate between Belgium and Germany, with associated costs covered by the project.

Desirable additional knowledge and experience:

- ML best practices, uncertainty quantification
- Δ-ML, applied ML experience for physics/chemistry
- Theory and simulation of IR/Raman/UV-VIS/X-ray spectroscopy
- Density functional theory, linear response theory, quantum mechanics
- Some experience with programming in a team, for a large-scale software package.
- Working knowledge of Fortran(90 - 2008) 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. The start date would be as soon as possible after 1 September. Salary and secondary benefits will follow EU rules for Doctoral Network Researchers:

- Supergross monthly living allowance: 3400 Euro / month.
- 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 partner institutions.

University of Liege offers 25 paid vacation days per year and flexible working hours as well as occasional remote work options.

The Host

About the nanomat group

The nanomat unit of the Physics Department at the University of Liège is a world-leading research group focusing on novel theories and software for the prediction of materials properties. The main thrusts are electron-phonon and phonon-phonon coupling with perturbation theory, nanostructured and defected materials, and magnetic dynamics including skyrmions and non-collinear textures. Nanomat is a core team of the abinit (www.abinit.org) open source software initiative, and constructs widely used databases and component libraries, such as the pseudo-dojo atomic potential sets (www.pseudo-dojo.org). We have close collaborations with other electronic structure theory in Physics, Chemistry and Engineering, and are embedded in strong networks, in particular psi-k (www.psi-k.net) and the European Theoretical Spectroscopy Facility (www.etsf.eu).

About University of Liège

The University of Liège is now 200 years old and one of the main universities in Belgium. It hosts a full spectrum of ten faculties with 45 departments, including medical and engineering schools. ULiège is home to 20000 undergraduate students (of which 4600 foreign students), 3000 academic staff, and 2000 PhD students. The main campus is on a forested hill outside town, in symbiosis with a local science park focusing on materials, IT, and space technologies. The University has pioneered open access repositories and has a full roster of e-learning and soft skills training sessions. ULiège received the award "HR excellence in research" (HRS4R) from the EU Commission in 2011. The University and city of Liège provide a rich and welcoming environment, with excellent infrastructure and amenities, reasonable cost of living, which is well connected by rail and plane to the rest of Europe.

Eligibility

We especially invite women and underrepresented minority group applications. Note that EU mobility rules apply (no more than 1 year residence in Belgium in the last 3). In principle, applicants can have any nationality and any current residence. Candidates who have already been awarded a PhD degree are not eligible.

Further information, applying

Detailed information can be found on the web for the nanomat group (http://nanomat.ulg.ac.be) and the University of Liège (www.uliege.be).

Key software involved in the project:

- The ABINIT package calculates ground and excited states of materials within DFT, DFPT, and MBPT

www.abinit.org

- The TDEP package calculates anharmonic thermal and transport properties:

ollehellman.github.io

- The SPRKKR package calculates spectroscopic and magnetic properties within a multiple scattering formalism

www.ebert.cup.uni-muenchen.de/index.php/en/software-en/13-sprkkr

Interested candidates are encouraged to contact us for further information. Job applications can only be sent by email to: Matthieu.Verstraete@uliege.be. The procedure will run until the position is filled. Applications should contain:

- CV
- Transcript of courses studied with grades and global ranking within your cohort
- 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).

It is finally the applicant's responsibility to ensure 2 reference letters are sent separately by email to the address above.