PREDICTOR

# JOB POSTING

## Recruiting organisation
Software for Chemistry & Materials B.V. (SCM)

## Subproject title
Improving the accuracy of solubility and solution-free energy predictions (COSMO-RS)

## Starting date
Between 1 July 2025 and 31 October 2025

## Salary
The Doctoral Network "PREDICTOR" is financed by the European Union under the framework of the program HORIZON Europe, Marie Skłodowska-Curie Actions. The doctoral candidate will be hired for 36 months under contract by Software for Chemistry & Materials B.V. with a starting monthly gross salary of approx. € 3426 (including mobility allowance, but excluding other allowances that depend on eligibility, e.g. family allowance, special needs allowance).

## Background information
Marie Skłodowska-Curie Doctoral Networks are joint research and training projects funded by the European Union. Funding is provided for doctoral candidates from both inside and outside Europe to carry out individual project work in a European country other than their own. The training network "PREDICTOR" is made up of 22 partners, coordinated by Fraunhofer ICT in Germany. The network will recruit a total of 17 doctoral candidates for project work lasting for 36 months.

PREDICTOR aims to establish a rapid, high-throughput method to identify and develop materials for electrochemical energy storage. It will enable the rapid identification, synthesis and characterization of materials within a coherent development chain, replacing conventional trial-and-error developments. To validate the PREDICTOR system, the case study will be active materials and electrolytes for redox-flow batteries. Within the project, three demonstrator battery cells (TRL3-4) will be assembled and tested with the newly developed materials.

## Our objectives:
- A **modelling and simulation tool** for the computational screening of organic chemicals based on their potential performance in energy storage systems.
- **Automated** chemical synthesis, electrolyte production and characterization methods, so that the chemicals identified in the screening step can be rapidly produced and tested for their suitability in energy storage applications.
- **Artificial- intelligence- based** self-optimization methods that allow experimental data from material characterization to be fed back into automated experimental methods to enable self-driving laboratory platforms and for modelling and simulation tools, improving their accuracy.
- **Data management systems** to standardize and store the data generated for further use in model validation and self-optimization processes.

## Job description
The advertized subproject is fully funded by the Marie Skłodowska-Curie European Training Network "PREDICTOR". It will be carried out by one doctoral candidate at Software for Chemistry & Materials B.V., with PhD supervision at RWTH Aachen University over a period of 36 months.

SCM is a scientific software company located in Amsterdam. We are passionate about computational chemistry and our customers are active in academia, government labs and industry worldwide studying various fields of chemistry and materials science.
We are looking for a PhD student to develop advance thermodynamic methods for accurately calculating solubility and solution free energy, with a particular emphasis on electrolyte systems. The focus is on improving and expanding SCM's existing methodologies, including COSMO-RS, Pitzer-Debye-Hückel, and machine learning (ML)-based approaches. The primary goal is to develop robust methodologies and software tools that facilitate more accurate calculations for electrolyte systems.
The position involves addressing key challenges such as refining general parameters that are relevant to both short-range interactions, as modelled by COSMO-RS, and long-range interactions, as described by Pitzer-Debye-Hückel models. Furthermore, the project seeks to integrate data-driven approaches to enhance ML-based models, thereby improving solubility predictions and estimating key physical properties that required the calculation framework.

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## Benefits

The recruited researcher will have the opportunity to work as part of an international, interdisciplinary team of 17 doctoral candidates, based at universities and industrial firms throughout Europe. She/he will be supported by two mentors within the PREDICTOR project, and will have multiple opportunities to participate in professional and personal development training. Through her/his work she/he will gain a unique skill-set at the interface between modelling and simulation, high-throughput experimentation / characterization and self-optimization and data management over different length scales from nano to the macroscopic level.

She/he is expected to finish the project with a PhD thesis and to disseminate the results through patents (if applicable), publications in peer-reviewed journals and presentations at international conferences.

## About SCM

Software for Chemistry & Materials B.V., SCM, is an independent spin-off company of the Vrije Universiteit Amsterdam, The Netherlands. 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 offers an informal working atmosphere in a small team of approx. 30 PhD-level researchers and scientific software developers from various nationalities and backgrounds. We offer our employees 34 paid holidays per year and flexible working hours, as well as occasional remote work options. All employees are enrolled in the ABP pension fund.

## Requirements

### Qualifications/experience:

- In accordance with the European Union's funding rules for doctoral networks, applicants must NOT yet have a PhD
- Knowledge of thermodynamic models, with a preference for candidates who have experience in COSMO-RS, COSMO-SAC and/or electrolyte modelling.
- Ability to comprehend the underlying physics of models presented in scientific literature, enhance these models, and efficiently translate them into source code.
- MSc in Physics, Chemistry, or a related science field.
- Good written and verbal communication skills in the English language.

### Desirable additional knowledge & experience

- Working knowledge of Fortran(90) and Python.
- Some experience with programming in a team, in a large-scale software package (>100,000 lines of code).
- 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.

### Mobility:

The applicant must not have resided or carried out her/ his main activity (work, studies etc.) in The Netherlands for more than 12 months in the past 3 years.

## How to apply

Applications can only be processed by filling out the webform on our website. The application procedure will continue to run until the position is filled, and new applications are welcomed.
https://www.scm.com/company/careers
https://www.scm.com/news/job-opening-marie-curie-phd-fellowship-cosmo-rs-thermodynamics-for-electrolytes/

***Application deadline***: 15th June 2025