EUSpecLab Doctoral Network
PhD positions

The ***EUSpecLab*** network is a Horizon Europe Marie Curie network centered on *Spectroscopies and Machine Learning*. It is due to start in September 2022 (month M1). We will propose 11 PhD positions in the EU and in Switzerland. The interview of the candidates are planned to start at the beginning of September, but candidates should apply as soon as possible.

We will propose 10 EU-funded PhD grants + 1 Swiss-funded one. The EU-funded projects are essentially theoretical ones.

Gross living allowance	3400 € / month * **SC**
Mobility allowance	600 € / month
Family allowance	660 € / month

The mobility allowance is due to all doctoral fellows. It covers their additional, private mobility-related costs (e.g. travel and accommodation costs), not their professional costs under the action, which are covered by the research, training and networking contribution.

The family allowance will be given to all researchers who have a family (regardless of whether the family will move with the researcher or not). The family obligation refers to persons linked to him/her by (i) marriage, or (ii) a relationship with equivalent status to a marriage recognised by the legislation of the country or region where this relationship was formalised; or (iii) dependent children who are actually being maintained by the researcher.

The effective gross living allowance is scaled by a factor depending on the country:

Researcher number	Country	Scaling coefficient SC
Researcher 1	France	116.4 %
Researcher 2	Czech Republic	79.1 %
Researcher 3	Belgium	100 %
Researcher 4	Finland	119.5 %
Researcher 5	Italy	97.4 %
Researcher 6	Sweden	125.4 %
Researcher 7	Denmark	132 %
Researcher 8	Germany	98.3 %
Researcher 9	Netherlands	109.6 %
Researcher 10	Austria	106.3 %

The acronyms used in the project description refer to the different members of the consortium listed after the description of the projects.

(i) EU-funded projects:

Fellow	Host institution			Place:	Rennes (France)
Researcher 1	**CNRS**			**Contact:**	**Didier Sébilleau didier.sebilleau@univ-rennes1.fr**

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 the **UT** partner is a full-potential spin-independent XAS code. The Researcher will include spin-polarization, in order to access the magnetic structure and strongly correlated systems. More precisely:

• Spin-polarised relativistic multiple scattering module for MsSpec and FPMS
• Full potential module for MsSpec (through **UT** secondment)
• Interface with state-of-the-art electronic structure codes (DFT, GW, …), through **UU** and **VUA** secondment.
• DMFT read-in or built-in to treat correlations (for low kinetic energies) (through **UWB** secondment).
• Testing against experimental data provided by **UWB** and **PSI**.
• Structure optimisation using machine-learning for the comparison between calculated and experimental spectra (based on **SCIENTA** secondment for the knowledge of how experimental spectra are treated) and **in collaboration with Researcher 11**

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.

Planned secondment(s): 10 months

* **UWB**, M30-M32; (1) incorporate correlation effects through DMFT (J. Minár), (2) perform spin-polarised photoelectron diffraction measurements (L. Nicolai).
* **UU**, H. Herper, M12; interface with ab initio molecular electronic structure, (codes: RSPt, Vasp+Quantum Espresso)
* **UT**, K. Hatada, M17-M18: merger of the potential generation part of MsSpec with that of FPMS
* **VUA**, L. Visscher, M13; interface with ab initio molecular electronic structure (code: ADF)
* **Intersectoral: SCIENTA**; M20-M22: acquire knowledge on the software used in photoemission data analysis

Enrolment in Doctoral degree(s): Université de Rennes-1

Fellow	Host institution			Place:	Pilsen (Czech Republic)
Researcher 2	**UWB**			**Contact**	**Ján Minár jminar@ntc.zcu.cz**

Electronic structure of lanthanide-doped materials for phosphor-converted white light emitting diodes

Objectives: 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.

Planned secondment(s): 9 months

AALTO: P. Rinke, M12-M13; understanding of deep learning models and setting up database for pcLED relevant materials.

UL: M. Verstraete, M22-23; implement ML for displacements and apply thermal property calculations to the emission quenching.

CNRS: D. Sébilleau, M30-M31; use of complementary spectroscopy methods (EELS) and photoelectron diffraction (PED) developed in the MsSpec package.

Intersectoral: RVM: R. Varga, M16-M18; Contact with experimental and theoretical tools in an industrial setting for disordered materials screening.

Enrolment in Doctoral degree(s): University of West Bohemia

Fellow	Host institution			Place:	Liège (Belgium)
Researcher 3	**UL**			**Contact:**	**Matthieu Verstraete Matthieu.Verstraete@uliege.be**

Vibrational and disorder effects in electronic and X-ray spectroscopy

Objectives: Experiments are now so precise that they challenge static and idealized theories. We will push the limits of spectroscopic simulations with realistic materials models. The central challenges today are to include a material's environment and disorder, whether thermal, chemical or structural. As full *ab initio* calculations are very heavy, either with explicit supercells or perturbation theory, we will "machine learn" 1) intermediate quantities such as mean square displacements and 2) the final shifts and linewidths of the spectrum, from a limited set of data points.

• Include thermal and chemical disorder effects in Xray and Transmission Electron Microscopy (TEM) simulations (in particular holography...). Train ML models to add these effects to "bare" calculations, based on chemistry and structure

• Develop a general theoretical framework for coherent (e.g., phonons, controlled doping) and incoherent (temperature, random alloying, vacancies...) perturbations in photon and electron spectroscopies.

• Applications to 2D materials and surfaces, including magnetic systems, e.g., CrI3, transition metals, and chalcogenides.

Expected Results:

1. Machine learning algorithm for the vibrational mean square displacement (MSQD) and other thermodynamic quantities, based on existing databases, ab initio MD, and NN potentials (with **MLU).**
2. Extension to anharmonic lattice dynamics using the Temperature Dependent Effective Potential method.
3. Comparison of the Coherent Potential Approximation (CPA) and Molecular Dynamics, and development of perturbation theory schemes beyond the Debye Waller approximation.
4. Inclusion of vibrational and thermal effects in X-ray spectroscopies and TEM.
5. Anisotropic/anharmonic MSQD as input for the CPA KKR (with **UWB**) in complex materials, surfaces and interfaces.
6. Realistic prediction of STEM maps with a dynamical and/or thermalised electron potential (with DrProbe or QSTEM).

Planned secondment(s): 6 months

* **Intersectoral: TME:** Hannah Johnson M18-M20; investigate the vibrational and thermal properties of MoSx matrices for Hydrogen Evolution Reaction catalysis

* **MLU:** M Marques, M12-14; to integrate ML tools for environmental (in particular vibrational) effects on spectroscopy

Enrolment in Doctoral degree(s): Université de Liège

Fellow	Host institution			Place:	Aalto (Finland)
Researcher 4	**AALTO**			**Contact:**	**Patrick Rinke patrick.rinke@aalto.fi**

Machine-learning based interpretation of infrared spectroscopy in heterogenous catalysis

Objectives: To develop a data-driven approach for analysing infrared spectra of in-situ catalyst characterization. Heterogeneous catalysis is an important industrial process for the production of chemical compounds and the conversion of chemicals (in e.g., car exhausts). Infrared spectroscopy is one of the characterization techniques that can provide in-situ and real-time information on catalyst operation. To facilitate spectra interpretation with the required quantum mechanical insight but without its high computational cost, we will develop a machine-learning model based on DFT data. We will adapt a recently developed global atomic structure descriptor and a regression model and parameterize it for platinum and rhodium catalysts. We will then predict the infrared spectra of chemical species (e.g., CO, CO_2, NO_x, H_2O and their reaction intermediates) and develop a deconvolution tool with our collaborators for the analysis of in-situ and operando spectra.

- Generate high-throughput DFT data sets for structure-spectra mapping
- Adapt our recently developed global machine-learning model for atomic structures to infrared spectra and validate it for catalysts
- Generate dataset of infrared spectra for reactants and reaction intermediates
- Develop spectra analysis tool

Expected Results:

- Large materials datasets for data driven catalysis and machine learning
- Machine-learning model for fast infrared spectra predictions of catalyst materials
- Spectra deconvolution tool for real-time analysis of in-situ experiments

Planned secondment(s): 7 months

* **Intersectoral: TME:** H. Nguyen, M24-26; application of spectral analysis tool in R&D
* **Academic MLU:** M18-20 methodological exchange and comparison of ML-based vibrational spectroscopy approaches

Enrolment in Doctoral degree(s): Aalto University

Fellow	Host institution			Place:	Camerino (Italy)
Researcher 5	**UNICAM**			**Contact:**	**Angela Trapananti angela.trapananti@unicam.it**

Reverse Monte Carlo atomistic structural modelling of materials constrained by X-ray absorption spectroscopy

Objectives: The main goal is the experimental study of the microscopic structure of materials by X-ray absorption spectroscopy (XAS). The project will address disordered systems such as oxide and chalcogenide glasses at different pressure-temperature conditions and hydrogen charged metals. This objective will require the further development of a data analysis approach based on Reverse Monte Carlo to build three-dimensional structural models having the best agreement with one or more sets of experimental data (XAS but also complementary wide and small angle x-rays and neutron scattering).
The Researcher will:
• develop and implement suitable computational strategies (and the related codes) to include wide/small angle scattering data, coordination constraints and/or ab-initio calculated multiple scattering EXAFS signals within the RMC modelling (implementation of genetic and machine learning algorithms to enhance the sampling efficiency will be explored).
• validate the approach and the developed code modules on test cases such as simple molecular systems
• perform and interpret X-ray absorption experiments on specific systems, such as prototypical oxide and chalcogenide glasses at different conditions of pressure and temperature
• in the framework of an intersectoral secondment, explore the capabilities of the approach to investigate local-medium range structure effects on steels or tungsten samples charged with hydrogen of interest for industrial applications (H reservoirs, fusion reactors).

Expected Results: • New data-analysis approaches (and related codes) for XAS of molecular and disordered systems based on Reverse Monte Carlo (inclusion of MS signals, constraints on the molecular structure and combined refinement with small angle scattering signals).

1. Validation of the approach on simple molecular systems.
2. New knowledge about the evolution of the atomic and electronic structure of prototypical glasses also under extreme conditions
3. Application to a specific industry relevant problem such as the investigation of changes of the short and medium range structure (phase changes, local distortions...) induced by hydrogen on steels and their correlation with microstructure damage

Planned secondment(s): 7 months

*** Univ. Toyama**: K. Hatada; M16-M18; to learn the fundamentals of multiple scattering calculations in X-ray absorption spectroscopy for its implementation in the RMC code
*** AALTO**: T. Rossi; M20; to learn ML methods and explore integration into Reverse Monte Carlo modelling
*** Intersectoral**: **RINA**: E. Zanin; M28, M32-M33; to develop knowledge of the industrial R&D on hydrogen charged steels or tungsten. Preparation of samples and TEM/SEM characterizations.

Enrolment in Doctoral degree(s): University of Camerino

Fellow	Host institution			Place:	Uppsala (Sweden)
Researcher 6	**UU**			**Contact:**	**Heike Herper heike.herper@physics.uu.se**

New functional Ce-based materials from materials design

Objectives: Ce-based materials are used in a large variety of applications whereby the oxidation state of Ce and the localization degree of the Ce 4f state largely determine the material properties. Using materials informatics to analyse data sets for a large collection of compounds to search for trends in materials classes. The goal of this project is to derive a method which allows to classify existing Ce systems and derive descriptors for high throughput searches to identify new materials with tailored properties for different applications (e.g. magnetic, thermoelectric, catalytic). XPS and XAS are important tools for the analysis and will be calculated for the systems under investigation. The level of theory needed depends on the localization of the (f) electrons and must be determined in a first step. Therefore, the following tasks will be addressed:
Performing DFT calculations to get electronic structure and hybridization function for determination of localization.

- Determination of the XPS and XAS (XMCD) using first principles techniques based on density functional theory (DFT) and/or dynamical mean field theory (DMFT) or SPRKKR (for alloys).
- Extension of the Uppsala full-potential LMTO code RSPt such that d-f transitions ($M_{4,5}$) edges can be handled (so far only p to d). Testing and comparison to available experimental spectra data

Expected Results:

· Extended and improved computer code RSPt to handle L and M edge spectra of correlated systems.
· Derivation of suitable descriptors to be used in High throughput calculations/machine learning to identify new candidate phases with tailored properties.
· Detailed insight in spin structure and electronic properties of newly predicted Ce-systems .

Planned secondment(s): 8 months

Academic: UWB, Jan Minár; M15-M16; gain expertise in SPR-KKR for calculation of XAS/XMCD for disordered systems.
Academic: DTU, K. Thygesen, M22-M23 machine learning techniques for analysis of the spectra, XAS
Intersectoral: SCIENTA, A. Hahlin, M31-M34, Analysis of the state-of-the-art file formats used in spectroscopy in industry and academics

*** Enrolment in Doctoral degree(s):** University of Uppsala

Fellow	Host institution			Place:	Copenhagen (Denmark)
Researcher 7	DTU			Contact:	Kristian Thygesen thygesen@fysik.dtu.dk

High-throughput spectroscopy of quantum point defects

Objectives: To develop an efficient theoretical framework for calculating the absorption and photoluminescence (PL) spectrum of point defects in insulating crystals and use it to perform a high-throughput characterisation of 1000 crystal/defect systems with the aim of identifying candidates for quantum technology applications (qubits, magnetic field sensing, and single photon sources). Since most applications of point defects in quantum technology takes advantage of the electron spin, we shall be most interested in defects that exhibit magnetic ground state and feature long spin coherence times. We will attempt to build machine learning models to predict key spectroscopic properties from simple chemical/structural features. The specific objectives are:

- Generate a computational database with relaxed structures for 1000 crystal point defects
- Identify defects with a high-spin ground state and small reorganisation energies
- Calculate the absorption and PL spectrum for the lowest optically active transition in the defects selected in the previous step
- Train a machine learning model on the database to predict PL spectra and magnetic states using simple structural fingerprints

Expected Results:

- A computational workflow for characterisation of the atomic and electronic structure of point defects
- A database with structural, energetic, and spectroscopic properties of crystal point defects
- A set of specific crystal/defect candidate systems with optimal properties for application as single-photon sources and solid-state qubits, respectively.

Planned secondment(s): 6 months

*** Intersectoral: SCM,** Prediction of PL spectra of point defects using machine learning techniques developed for molecules. M18-20.
*** Academic: MLU,** Prediction of PL spectra of point defects using machine learning techniques developed for interfaces. M24-26.

Enrolment in Doctoral degree(s): Technical University of Denmark

Fellow	Host institution			Place:	Halle (Germany)
Researcher 8	**MLU**			**Contact:**	**Miguel Marques miguel.marques@physik.uni-halle.de**

Vibrational spectroscopy of complex systems from neural network force fields

Objectives: This project will develop a machine-learning software to simulate spectroscopic properties of interfaces with neural-network force fields using analytical second-derivatives. This will allow for a numerically precise method (much more than a frozen-phonon approach) capable of delivering the vibrational frequencies of systems with thousands of atoms with DFT quality. This tool will then be used to investigate the localized vibrational modes of several interfaces. We will then extend our software to provide the analytical third-order derivatives that open the door for the investigation of thermal transport properties and of Raman spectra. The energetically favoured interface reconstructions will be efficiently identified by crystal structure prediction, using machine learning force fields, together with a constrained variant of the minima hopping method. Electronic band diagrams across the interface will also be calculated using density functionals for interfaces, developed and tested in Jena.

The specific objectives are:

- Software development: vibrational and phonon spectrum from analytical differentiation of the neural network.
- Software development: third derivatives and calculation of thermal transport coefficients.
- Training of neural-network force fields for the study of few paradigmatic systems also studied by **Researcher 7.**
- Apply neural-network force fields, to further speed up calculations of realistic atomic structures of interfaces. A library of force fields, that can provide accurate energies and forces, covering the whole periodic table is necessary for this task.
- Study of phonon scattering by interfaces.

Expected Results:

- Software tool to calculate vibrational and thermal properties from neural-network force-fields. This tool will be open-sourced and integrated with existing software.
- Raman spectrum of point defects that can be directly used for the understanding of experimental data.
- Understanding and quantitative evaluation of the phonon scattering at point defects and interfaces.

Planned secondment(s): 6 months

*** Intersectoral: TME**; M18-M20; training on ML force fields for structural prediction of vibrational spectra of interfaces.
*** Academic: DTU**, K.S. Thygesen; M30-M32; learning on physics and simulation of defects in bulk materials, aiming to extend the study to defects at interfaces and interface functionalization through control of defects.

Enrolment in Doctoral degree(s): Martin Luther University Halle

Fellow	Host institution			Place:	Amsterdam (Netherlands)
Researcher 9	**SCM**			**Contact:**	**Stan van Gisbergen vangisbergen@scm.com**

Predicting optical and vibrational spectra for molecules from ML-enhanced DFT

Objectives: The Researcher at **SCM** will develop and apply new methods to apply machine-learning (ML) techniques to predict spectroscopic properties of molecules. Initially we will focus on vibrational (such as IR) and optical (UV-Vis) properties, with possible later extensions to magnetic and chiral properties. These properties are currently calculated with DFT in ADF and, for some, with the faster but more approximate DFTB method.

The new methods will either focus on direct prediction of spectra, bypassing DFT altogether, or focus on hybrid DFT (or DFTB) / ML methods to improve current spectroscopic predictions in either speed or quality. This will be done by delta-ML methods to train a neural network on the difference of Fock matrix in the ground state for DFT (in some suitably localized basis set) and DFTB as well as on matrices related to perturbed 1st-order Fock matrices relevant for response properties. The ML methods will also be developed by using the expertise in Optimal Transport (OT) theory of the Theoretical Chemistry **VUA**, for example by using its distance metric to define differences between spectra.

1. Develop methods, to be implemented in **SCM'**s software suite, for improved spectra prediction of molecules, using ML and OT, starting from geometry and/or fast DFTB-based spectra
2. Develop ML-based methods inside **SCM**'s DFT(B) codes to improve the matrices needed to calculate the spectra

Expected Results:

1. ML-based method to predict optical and vibrational spectra for molecules directly from geometry
2. Improved DFTB molecular spectra by training difference between DFT and DFTB matrices

Planned secondment(s): 6 months

Intersectoral (academic):

1. **AALTO**, P. Rinke, M10-M12: training on ML techniques.
2. **JENA** S. Botti, M20-M22: joint application of vibrational spectra methods on interfaces.

Enrolment in Doctoral degree(s): Vrije Universiteit Amsterdam

Fellow	Host institution			Place:	Vienna (Austria)
Researcher 10	**TUW**			**Contact:**	**Wolfgang Werner werner@iap.tuwien.ac.at**

X-ray Photoelectron Spectroscopy Data Analysis using a Neural Network

Objectives: We plan to develop an algorithm based on a neural network to improve data analysis of X-ray photoelectron spectroscopy data for chemical surface analysis. The neural network will be used to improve data quality and do element and compound classification. For the element and compound classification we plan to use SESSA (Simulation of Electron Spectra for Surface Analysis) to generate artificial XPS data for training the neural network. The +30.000 experimental XPS at NIST as well as new data taken **TUW**, **PSI**, and **SCIENTA** will be used for test purposes. The specific objectives are:

- Installing and developing a neural network for spectral data analysis.
- Installing a software interface to SESSA and generating >100.000 test data.
- Training of the neural network.
- Testing of neural network with experimental data from NIST, **TUW**, **PSI**, and **SCIENTA**.

Expected Results:

- Neural network suitable for XPS data evaluation.
- Generating proper training data and testing of the accuracy of the neural network.
- Software package for elemental and compound classification using the neural network.

Planned secondment(s): 9 months

*** Intersectoral:**
SCIENTA: M9-11, gain insight in ARPES and STM experiments and corresponding software
*** Academic:**
UU, Heike Herper**.** 20-22 Apply neural network software to analysis of Ce-based materials
PSI, Matthias Muntwiler. M16-18 Hands-on experience of photoemission at a synchrotron. Influence of photoelectron diffraction on the shape of XPS spectra

Enrolment in Doctoral degree(s): TU Wien

(ii) Swiss-funded project:

Fellow	Host institution			Place:	Villigen (Switzerland)
Researcher 11	**PSI**			**Contact:**	**Matthias Muntwiller matthias.muntwiler@psi.ch**

Detailed adsorption geometry of magnetic molecules under weak and strong binding conditions

Objectives: This project investigates the influence of adsorption geometry on magnetic interactions of porphyrin-based single-ion magnetic molecules with the underlying substrate. X-ray magnetic dichroism measurements show clear differences in magnetic exchange coupling including a cross-over from ferromagnetic to antiferromagnetic order in different adsorption configurations. Precise and reliable experimental data on the adsorption geometry (adsorption height, in particular) are, however, lacking due to the complexity of molecular systems. In this project, synchrotron-based angle- and energy-scanned photoelectron diffraction in connection with multiple-scattering calculations enhanced by machine-learning techniques will be used as a sensitive probe of the local structure around the magnetic centre of the molecule. A major part of the project shall be the development of efficient structural optimization code that will be able to handle the complexity of adsorbed organic molecules. This will be done by complementing existing optimization code with scattering code developed in WP1 and machine learning techniques developed in WP2 of the network.

Key features of the new code:

1. Interface to scattering code developed within the DN.
2. Make structural optimization more efficient by using machine-learning techniques to quickly categorize a parameter vector as compatible or incompatible with measurement.
3. Reduce the number of parameter dimensions by automatically identifying and separating significant parameters.
4. Interface with first-principles codes to (1) import electronic potentials for calculating scattering factors and (2) verify specific models for compatibility with theory.

Expected Results:

1. An uncomplicated, efficient and well-documented data analysis workflow for solving complex surface structures by leveraging machine-learning techniques and first-principles theory developed in the EuSpecLab network for the simulation of photoelectron diffraction patterns.
2. Experimental determination of the adsorption geometry of magnetic porphyrins on magnetic surfaces and their influence on magnetic interaction strength and cross-over phenomena.

Planned secondment(s): 6 months

* **Academic: CNRS**: D. Sébilleau; M12-14; Training on the basic photoelectron diffraction code
* **Intersectoral: PINFLOW:** Jiri Varna M22-M24; modifications of surface of the electrodes studied by PED and XPS

Enrolment in Doctoral degree(s): University of Basel

Composition of the Consortium

Consortium Member	Legal Entity Short Name	Academic	Non-academic	Awards Doctoral Degrees (tick)	Country	Dept./ Division / Laboratory	Scientist-in-Charge	Role of associated Partner or link to beneficiary
Beneficiaries								
1.Centre National de la Recherche Scientifique	CNRS	✓			FR	Inst. de Physique de Rennes	Dr. Didier Sébilleau	
2. University of West Bohemia	UWB	✓		✓	CZ	New Technologies Research Centre	Prof. Ján Minár	
3. Université de Liège	UL	✓		✓	BE	Dept of Physics	Prof. Matthieu Verstraete	
4. Aalto University	AALTO	✓		✓	FI	Computational Electronic Structure Theory	Prof. Patrick Rinke	
5. University of Camerino	UNICAM	✓		✓	IT	School of Science and Technology	Dr. Angela Trapananti	
6. University of Uppsala	UU	✓		✓	SE	Dept of Physics and Astronomy	Dr. Heike Herper	
7. Technical University of Denmark	DTU	✓		✓	DK	Department of Physics	Prof. Kristian Thygesen	
8. Martin-Luther Universität Halle-Wittenberg	MLU	✓		✓	DE	Institut für Physik	Prof. Miguel Marques	
9. Software for Chemistry & Materials BV	SCM		✓		NL		Dr. Stan J.A. van Gisbergen	
10. Technical University Vienna	TUW	✓		✓	AU	Institut for applied physics	Prof. Wolfgang Werner	
Associated Partners								
11. Paul Scherrer Institut	PSI	✓			CH	Photon Science Division	Dr. Matthias Muntwiler	Secondments and researcher #11
12. Centrum Dohody	CEDO		✓		CZ		Alice Hamplová	Training
13. European Multifunctional Materials Institute	EMMI		✓		BE		Prof. Jean Étourneau	Training
14.Pinflow energy storage, s.r.o.	PINFLOW		✓		CZ		Dr. Jiri Vrana	Training and secondments
15.RVMagnetics	RVM		✓		SK		Prof. Rastislav Varga	Training and secondments
16.Vrije Universiteit Amsterdam	VUA	✓		✓	NL	Department of Chemistry and Pharmaceutical Sciences	Prof. Paola Gori Giorgi	Training and secondments
17.University of Toyama	UT	✓		✓	JP	Faculty of Science	Prof. Keisuke Hatada	Training and secondments

18.Friedrich Schiller Universität Jena	JENA	✓		✓	DE	Institut für Festkörpertheorie und -optik	Prof. Silvana Botti	Training and secondments
19.Toyota Motor Europe NV	TME		✓		BE		Dr. Konstantinos Gkagkas	Training and secondments
20.Rina Consulting	RINA		✓		IT		Dr. Egidio Zanin	Training and secondments
21.Scienta-Omicron	SCIENTA		✓		DE		Dr. Anders Hahlin	Training and secondments
22.Universität Basel	UB	✓		✓	CH	Department of Physics	Prof. Thomas Jung	PhD delivering
23.Université Rennes 1	UR1	✓		✓	FR			PhD delivering