

STUDENT MOBILITY FOR PLACEMENT
TRAINING AGREEMENT and QUALITY COMMITMENT/
PRACOVNÍ PLÁN A ZÁVAZEK KVALITY
MOBILITY PROGRAM ERASMUS MOBILITY FOR PLACEMENT

I. DETAILS OF THE STUDENT

Name of the student: Pavel Ondračka	Country: CZECH REPUBLIC
Home university: MASARYK UNIVERSITY	Academic Year: 2013/2014
Home university field of study: Physics	Subject area: Physics 13.2 Degree: MSc degree programme, full-time study mode

II. DETAILS OF THE PROPOSED TRAINING PROGRAMME ABROAD

Host organisation: <i>Montanuniversität Leoben</i>	
Address: <i>Franz Josef-Straße 18, Leoben 8700, Austria</i>	
Size of the host organisation:	<input type="checkbox"/> S = Small (1- 50 staff) <input type="checkbox"/> M = Medium (51-500 staff) <input checked="" type="checkbox"/> L = Large (>500 staff)
Type of work placement sector: Research	

Planned dates of start and end of the placement period: from 1. 9. 2013 to 30. 8. 2014 that is 12 months.

Knowledge, skills and competence to be acquired:

Pavel Ondračka is currently finishing his Master Studies in the field of physics. His thesis, supervised by Assoc. Prof. Lenka Zajíčková, deals with the plasmachemical deposition of hydrogenated carbon films and their characterization by optical methods in wide spectral range. The main part of the thesis focuses on the fitting of optical data by advanced dispersion models based on the parametrization of density of states. Pavel Ondračka will finish his thesis and obtain MSc. title in June 2013. Afterwards, he will start his PhD thesis under the supervision of Assoc. Prof. Lenka Zajíčková in the PhD study program Advanced Materials and Nanoscience. The suggested research programme aims to extend his expertise in quantum mechanical calculations of structural, electronic and optical properties of materials using the state-of-the-art implementations of the Density Functional Theory (DFT).

During his stay at Montanuniversität Leoben, Pavel Ondračka will get familiar with performing DFT calculations, working under Linux operating system. He will become aware of the possibilities and limitations of standard DFT methods, and how these can be overcome. He will gain knowledge on first principle calculations of the optical spectra which will well complement his current knowledge on the experimental side of the topic.

Through the regularly scheduled reports Pavel Ondračka will gain proficiency in scientific writing, which he will subsequently use in preparing a manuscript summarising all his calculated results.

Finally, by living abroad and working in an enthusiastic, friendly internationally competitive environment, Pavel Ondračka will gain awareness of the living conditions in other European country, will improve his English and develop German language skills.

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Detailed programme of the training period:

The work will focus on *ab initio* calculations of structural and optical properties of various oxide systems using the Density Functional Theory (DFT). State-of-the-art simulation packages employing local density approximation (LDA) and generalised gradient approximation (GGA) for the exchange-correlation potentials will be used. In the first stage, Pavel Ondračka will gain basic experience with the capabilities and limitations of the DFT technique, and through a hands-on approach will get familiar with two codes, Wien2k and SIESTA, that will be used in the study. Ground state properties of various TiO_2 and HfO_2 phases will be calculated, and will be benchmarked against available experimental and calculated results from the literature. The main scientific highlight of Pavel's work will be the calculation of optical properties (dielectric function) and electron energy loss near edge structures (ELNES) of selected material allotropes. These can be directly correlated with the experimental results obtained by the group of Assoc. Prof. Lenka Zajíčková in Brno. Furthermore, they can be used as a finger-print technique for allotrope identification of materials with the same chemistry (e.g., to distinguish between rutile and anatase phases of TiO_2). Time permitting, an attempt to address alloying-related issues and/or calculate properties of amorphous phases will be made.

Work plan

Task 1 (2 months)

Introduction to DFT, getting familiar with Linux operating system and the structure of Wien2k and SIESTA codes

Literature survey on the topic of structural and optical properties of TiO_2 and HfO_2 allotropes

Output: Short report on what has been done so far

Task 2 (4 months)

Convergence tests (optimisation of the calculation procedure)

Structural optimisation (equilibrium lattice parameters, enthalpy of formation, ground state electronic structure) of the selected oxide allotropes

Output: Report on ground state structural and electronic properties

Task 3 (4 months)

Calculation of dielectric functions for selected material systems

ELNES of relevant edges

Output: Written report on the optical properties and ELNES

Task 4 (2 months)

Dissemination of the results – preparation of a manuscript

Advanced topics (alloying, amorphous phases, etc.)

Output: Manuscript submitted to a peer-reviewed journal

Tasks of the trainee:

- Literature survey of state-of-the-art in the field of calculation of optical and electronic properties of binary Ti-O and Hf-O systems
- Mastering DFT codes
- Performing benchmark structural calculations
- Calculation of optical properties and ELNES spectra
- Preparation of a manuscript for the submission to a peer-reviewed journal

To be able to perform the tasks, the minimum level of language competence expected from the trainee in the main working language(s)¹ that the trainee will use at the host department/organisation (as define under point III) is:

	reading	speaking	writing
English	advanced	advanced	intermediate

In case the placement takes place in a representation or public institution of the home country of the student (e.g. cultural institutes, schools) please indicate the additional transnational benefits the student will obtain as compared to a similar placement in his or her home country. Placements in a national diplomatic representation (embassy and consulate) of the home country of the student are not authorised:

Is this placement fully integrated in the curriculum of the trainee's degree: ☒ YES ☐ NO

Monitoring and evaluation plan:

On a daily basis, Pavel Ondračka will be supervised by Dr. David Holec, leader of the Materials Modelling group at the Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben. Upon finalising each of the four stages of the work programme, Pavel Ondračka will prepare a short written report and/or a presentation. These will be provided to his supervisor at MU Brno, Assoc. Prof. Lenka Zajíčková, and will serve as a basis for discussion on the follow-up steps. Video-conferences between Montanuniversität Leoben and MU Brno and/or personal meetings in Brno or in Leoben will be organised for the purposes of mutual communication on the research progress. Additionally, Pavel Ondračka will present his results during "Materials Club", a departmental seminar for PhD students at Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben. At the final stage, the findings will be disseminated as a regular article in a peer-reviewed journal.

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¹ e.g., basic/intermediary/advanced/fluent in reading/speaking/writing. More precise references may be used, notably CEFR.



III. COMMITMENT OF THE THREE PARTIES

By signing this document the student, the sending institution and the host organisation confirm that they will abide by the principles of the Quality Commitment for student placements set out in the document below.

The student:

Student's signature: *Paul Chabala*

Date: *7.3.2013* (dd.mm.yyyy)

MASARYK UNIVERSITY (home institution):

We confirm that this proposed training programme agreement is approved. On satisfactory completion of the training programme Masaryk University will give recognition of completion of a Placement abroad course (code: *XD103*) and award the student with the following number of ECTS credits: *30*

Form of recognition at MU: C

Indicate by entering the letter (A, B, C) the form of recognition at Masaryk University: Choose from "A" for compulsory course recognition / *uznání jako povinný předmět*, "B" for selective course recognition / *uznání jako povinně-volitelný předmět*, or "C" for elective course recognition / *uznání jako volitelný předmět*. If not decided yet enter / *nerozhodnuto, vložte „-“*.

Student will be given a record of the training period in the Diploma Supplement.

The placement is compulsory part of study programme curricula: ☒ YES ☐ NO

Coordinator's name and function:

Date: *7.3.2013* (dd.mm.yyyy)

Asoc. Prof. Lenka Zepířková

Coordinator's signature: *[Signature]*

The host organisation:

We confirm that this proposed training programme is approved. On completion of the training programme the organisation will issue a Confirmation of placement period.

The student will receive a financial support for his placement from our sources: ☐ YES ☒ NO

The student will receive a contribution in kind for his placement from our sources: ☐ YES ☒ NO

Name and position of the mentor (if not available, the name shall be communicated to the student upon his/her arrival): Dr. David Holec

Normal working hours/week (overtime should no be the rule): 40

Number of permanent staff in the department (team) hosting the student: ~20

Number of other students/trainees hosted at the same time in the department (team) hosting the student: ~50

Is the student covered by the accident insurance of the host organisation (covering at least damages caused to the student at the workplace):

☒ YES (accident insurance nr: A 56 404 35 24 insurer: Allianz Elementar Versicherungs-AG) ☐ NO

If yes, please specify if it covers also:

- accidents during travels made for work purposes: ☐ YES ☒ NO

- accidents on the way to work and back from work: ☒ YES ☐ NO

Is the student covered by a liability insurance of the host organisation (covering damages caused by the student at

the workplace):

☒ YES (liability insurance nr: A 56 404 35 24 insurer: Allianz Elementar Versicherungs-AG) ☐ NO

Coordinator's name and function:

Date: ...06.03.2013.... (dd.mm.yyyy)

Prof. Helmut Clemens

Head of the Department of Physical Metallurgy and
Materials Testing

Coordinator's signature: 

QUALITY COMMITMENT for Erasmus placements

MASARYK UNIVERSITY* UNDERTAKES TO:

Define the **learning outcomes** of the placement in terms of the knowledge, skills and competencies to be acquired.

Assist the student in **choosing** the appropriate host organisation, project duration and placement content to achieve these learning outcomes.

Select students on the basis of clearly defined and transparent criteria and procedures and sign a **placement contract** with the selected students.

Prepare students for the practical, professional and cultural life of the host country, in particular through language training tailored to meet their occupational needs.

Provide logistical support to students concerning travel arrangements, visa, accommodation, residence or work permits and social security cover and insurance.

Give **full recognition** to the student for satisfactory completed activities specified in the Training Agreement.

Evaluate with each student the personal and professional development achieved through participation in the Erasmus programme.

MASARYK UNIVERSITY AND HOST ORGANISATION JOINTLY UNDERTAKE TO:

Negotiate and agree a tailor-made **Training Agreement** (including the programme of the placement and the recognition arrangements) for each student and the adequate mentoring arrangements.

Monitor the progress of the placement and take appropriate action if required.

THE HOST ORGANISATION UNDERTAKES TO:

Assign to students **tasks and responsibilities** (as stipulated in the Training Agreement) to match their knowledge, skills, competencies and training objectives and ensure that appropriate equipment and support is available.

Draw a **contract or equivalent document** for the placement in accordance with the requirements of the national legislation.

Appoint a mentor to advise students, help them with their integration in the host environment and monitor their training progress.

Provide **practical support** if required, check appropriate insurance cover and facilitate understanding of the culture of the host country.

THE STUDENT UNDERTAKES TO:

Comply with all **arrangements** negotiated for his/her placement and to do his/her best to make the placement a success.

Abide by the **rules and regulations** of the host organisation, its normal working hours, code of conduct and rules of confidentiality.

Communicate with the sending institution about any problem or changes regarding the placement.

Submit a report in the specified format and any required supporting documents at the end of the placement.