Project B2:
Astrochemistry in the atmosphere and winds of photoevaporating discs

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Requested positions: 1 Postdoc

Abstract:

Protoplanetary discs lose mass via a slow disc wind, probably driven by photoevaporation from the central star. A thermochemical study of this important component of in transition discs does not exist to date. The study of the chemistry in disc winds however relies on a knowledge of the opacities, which are largely dominated by small dust grains which are entrained in the wind from the underlying disc at the launch point. In this project we plan to develop a reduced chemical network appropriate for photoevaporative wind conditions and couple our chemical codes to space and time-varying dust distribution obtained in project C2. We will for the first time be able to draw detailed chemical profiles of photoevaporative winds and provide predictions by using radiative transfer codes, which is of fundamental importance to identify and interpret new spectral line diagnostics in existing and upcoming observations.

1. State of the art and preliminary work

Chemical models of gas in the protoplanetary and transition discs (TDs) are essential to pin down the initial conditions of the gas and dust from which planets form. Several sophisticated models have been and are continuously being developed to interpret the recent (e.g.) Herschel and ALMA observations of discs (e.g. Bruderer et al. 2015; Thi et al. 2013; Aresu et al. 2012; Meijerink et al. 2012; Woitke et al. 2010). These models however deal only with the dense parts of the discs, in rare cases extending to the bound disc atmospheres. Panoglou et al. (2012) have followed ionisation, chemical and thermal evolution within a steady state magneto-hydrodynamic disc wind solution and investigated various stages of young stellar objects (from Class 0 to Class II). No chemical model of a photoeveaporative TD wind as well as no time-dependent chemical model coupled with the dynamical evolution of a disc exist to date. This is a serious shortcoming for the identification of suitable wind tracers and more importantly wind diagnostics, to guide new observations and constrain disc dispersal models (see discussion in project B1).

The physical conditions valid for material in the bound disc itself are not appropriate at all for a disc wind. First of all winds are much less dense than the material in the bound discs. Even in the case of vigorous X-ray driven winds, the densities at the base of the wind are rarely above ten million hydrogen atoms per cubic centimetre, and they decrease roughly with the square of the distance (i.e. they behave roughly like Parker winds, see e.g. Owen et al. 2010; Font et al. 2004). The opacity in the wind is further reduced because of the decrease in dust content, as only a fraction of the grains contained in the underlying disc are entrained in the wind (see Owen et al. 2011b and discussion in project C2). For these reasons molecules may have a much shorter lifetime and indeed parts of

the gas in the wind will be completely photodissociated. For such physical conditions processes like surface chemistry, freeze-out etc. are not important, yielding a simpler problem, which bears less uncertainties compared with chemical models for colder and more opaque material in the bulk of the disc.

The chemical structure of the bound disc is however important to provide the initial conditions for the chemistry in the wind. It is also crucial to follow in detail the ionisation structure, as a recent paper by Wang & Goodman (2016) has pointed out that current estimates of ongoing accretion in TD systems are consistent with magnetized winds. Below, we describe the state-of-the-art in the field of disc chemistry and ionzation, where team members of Project B2 have played a crucial role.

Chemical models of protoplanetary discs

Gas and solid chemistry play a key role in the evolution of planet-forming discs and in planet formation theories, and determine the original composition of (exo)-planets (Henning & Semenov 2013). Planets are formed in protoplanetary discs that evolve over its typical lifetime of a few millions years (Fedele et al. 2010) by viscous spreading (e.g., Hueso & Guillot 2005; Baillié & Charnoz 2014) combined with photoevaporation (Alexander et al. 2013). During that time, the dust grains coagulate to each other to reach the size of meter- then kilometre- sized bodies (Birnstiel et al. 2010, 2012). Those bodies can agglomerate into planets or participate to the late episodes of heavy bombardments, bringing material onto planetary atmospheres and surfaces. Detection of the main belt asteroids reinforces the idea that asteroids may have brought most of the water on Earth (Jewitt 2012). Another key role played by chemistry is to set the location of the disc region where water is frozen onto solids, the so-called ice zone. Beyond the water ice zone, giant gas planets like Jupiter can form after the rapid accumulation of solid cores of 10 Earth masses by the core-accretion model (Helled et al. 2014, Öberg et al. 2015a, Helling et al. 2014).

Contrary to their young counterpart 'hot-corinos' (Cazaux et al. 2003), a much limited amount of molecules have been detected in protoplanetary discs. The outer disc molecular inventory includes CO, CN, HCN, formaldehyde, C_2H, CS, CH_3CN, HCO^+ and after a lot of effort CH_3OH (e.g. Dutrey et al. 2014; Öberg et al. 2015b; Walsh et al. 2016). The low abundance of many of the molecules has been ascribed to a combination of photodissociation at the disc surfaces and freeze-out onto grain surfaces towards the disc mid-plane. Simple molecules such as H_2, HD, CO, CO_2, H_2O, C_2H_2, HCN, N_2H^+, and potentially CH_3OH, have been detected from the terrestrial planet-forming region of protoplanetary discs by high-resolution spectrometers from ground-telescopes and by the Spitzer Space Telescopes (Pontoppidan et al. 2014). The gas is sufficiently warm such that many molecules are formed by neutral-neutral reactions with activation barrier. The ro-vibrational transitions in the mid-infrared have the advantage that homonuclear species such as CO_2 or C_2H_2 can emit contrary to pure rotational transitions. In addition to those small species, Polycyclic Aromatic Hydrocarbons (PAHs) infrared emissions are prominently seen from discs around the UV-luminous Herbig Ae stars. Carbonaceous compounds such as tholins may have been detected in an evolved disc (Debes et al. 2008, Köhler et al. 2008). The detected lines in both the inner and outer disc are emitted well above the mid-plane. Although the amount of detected species may be low, the chemical paths are not because of the large range of density, temperature, and UV field strength. Thermo-chemical disc models use a common unique network to model the entire disc. Many questions remain on the origin and survivability of complex organic molecules in protoplanetary discs in general and in the Solar Nebula in particular. We expect that grain surface thermal- and photoreactions (UV and X-ray) and high-energy particles play an important role in the formation of complex species in the disc regions where water can be frozen onto grains (Throop 2011, Ciesla & Sandford 2012, Walsh et al. 2014). The energetic radiations break molecular bonds producing reactive radicals and ions but stellar wind can inhibit the propagation of cosmic rays (Cleeves et al. 2013). Grain surfaces enhance considerably the probability for two species to meet and form other species. Throop (2011) and Ciesla & Sandford (2012) models do quantify neither the specific species that are synthesised nor their amount, but have demonstrated that complex organics can indeed form on the Solar Nebula grain surfaces. In addition Ciesla & Sandford (2012) results suggest that gas and dust transport in the Solar Nebula (and in

discs) will interconnect disc regions with dissimilar physical and chemical environments.

We are active collaborators within the ProDiMo[1] consortium (see e.g. Thi et al. 2014; Woitke et al. 2016). ProDiMo is a software package to model static protoplanetary discs including gas phase, X-ray and UV-photo-chemistry, gas heating and cooling balance, disk structure and (dust & line) radiative transfer. Surface chemistry has been recently included (Thi et al., in preparation).

Ionisation in discs

An accurate calculation of ionisation-recombination balance in dense protoplanetary conditions is essential for understanding various fundamental problems, such as coupling of the gas with magnetic field (Li et al. 2014), accretion processes (Turner et al. 2014), chemistry (Semenov et al. 2004; Larsson et al. 2012) and dust evolution (Okuzumi et al. 2011b; Akimkin 2015). The charging of grains in such environments affects their interaction of surrounding ions and electrons (Okuzumi 2009; Weingartner & Draine 1999) and hence modifies the chemistry at the grain surface.

Both the ionisation and recombination processes can arise from several sources. Primary agents of ionisation in dense gas (at visual extinctions above $A_{\mathrm{V}} \sim 10 - 30$ mag, where interstellar UV photons are absorbed) are X-rays, cosmic-rays (CRs), and the decay of radionuclides, leading to the ionisation fraction that decreases with density (Oppenheimer & Dalgarno 1974; Caselli et al. 2002; Maret et al. 2006). In discs around young, active stars the situation is complicated due to the presence of stellar X-rays (Glassgold et al. 1997) and the possible exclusion of low-energy CRs by protostellar winds (Cleeves et al. 2013b). Efficiency of stellar X-rays to ionize the circumstellar gas depends on the total fluxes and the hardness of the spectra (Igea & Glassgold 1999). Near the disc midplane, where X-rays and CRs are strongly attenuated, radioactive elements may substantially contribute to the electron fraction. In this case the ionisation rate is proportional to the abundance of the radioactive element and its decay rate (Umebayashi & Nakano 2009; Cleeves et al. 2013a): Short-lived radionuclides (SLR, mostly ^{26}Al with half-life 7.4×10^5 yr) contribute comparatively more than long-lived radionuclides (LLR, mostly ^{40}K with half-life 1.3×10^9 yr), but decay faster.

While the treatment of ionisation, despite the variety of ionisation sources, could be reduced to a single (total) ionisation rate, the description of recombination is less straightforward. At sufficiently high densities, where the dominant sink of free electrons and ions are dust grains, the recombination rate non-trivially depends on properties of the grains (Okuzumi et al. 2011a,b; Ivlev et al. 2016).

The grain charges are determined by different mechanisms operating in different regions of discs: In the disc atmosphere, the photoelectric emission from grains is a prominent charging mechanism, leading to positive charges (Weingartner & Draine 2001; Weingartner et al. 2006; Akimkin 2015). Not only stellar radiation, but also H_2 fluorescence induced by CRs can contribute to this (Ivlev et al. 2015). In the inner, midplane disc regions the photoemission becomes negligible, and the grain charges are determined by collection of electrons and ions from the surrounding weakly ionized gas, leading on average to negative grain charges.

Depletion of electrons in dense disc regions, caused by the presence of negatively charged grains, significantly reduces the degree of ionisation (Umebayashi 1983; Umebayashi & Nakano 1990; Nishi et al. 1991). As the ionisation controls the coupling of the gas to the magnetic field, and hence the development of the magnetorotational instability (MRI, e.g. Velikhov 1959, Balbus & Hawley 1991; Armitage 2015), dust is the essential ingredient for any MRI model. It has been shown that the grain size critically affects the size of a disc's "dead zone" (Sano et al. 2000; Salmeron & Wardle 2008; Bai 2011a,b; Dudorov & Khaibrakhmanov 2014).

Recently we have developed an exact analytical model which describes ionisation and dust charging in dense disc conditions, for arbitrary grain-size distribution (Ivlev et al. 2016). Unlike previously developed approaches (Ilgner & Nelson 2006; Okuzumi 2009; Fujii et al. 2011; Dzyurkevich et al. 2013; Mori & Okuzumi 2016), our model does not make assumptions on the form of the grain charge distribution, and enables convenient analysis of results in a general form, in terms of a few dimensionless numbers, which allows us to identify universality in the behavior of the charged species.

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[1]http://homepage.univie.ac.at/peter.woitke/ProDiMo.html

1.1 Project-related publications

Carmona, A. et al. 2014, A&A, 567, 51
Caselli et al. 1998, ApJ, 499, 234
Caselli et al. 2002, ApJ, 565, 344
Ivlev, A. et al. 2015, ApJ, 812, 135
Ivlev, A. et al. 2016, ApJ, in press (arXiv:1607.03701)
Keto, E. et al. 2015, MNRAS, 446, 3731
Szücs, L. et al. 2010, ApJ, 720, 1668
Szücs, L. et al. 2016, MNRAS, 460, 82
Thi, W.-F. et al. 2014, A&A, 561, 50
Woitke, P. et al. 2016, A&A, 586, 103

1.1.1 Articles published or officially accepted by publication outlets with scientific quality assurance; book publications

1.1.2 Other publications

[Text]

1.1.3 Patents

1.1.3.1 Pending

[Text]

1.1.3.2 Issued

[Text]

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The project will develop along a four-stage path of growing complexity. It is possible that some of the tasks in stage three may be carried over to the next funding period. The three stages can be described as follows:

1. **The reduced network.** A first task for this project is to simplify the gas-grain chemistry by reducing the chemical network to the minimum number of reactions needed to properly follow the formation/destruction of important species (in particular Hydrogen, Carbon, Oxygen as well as simple C-, O-bearing molecules) and the electron abundance or ionisation fraction. The PI of this project has extensive experience in devising efficient but reliable reduced networks (see e.g. Keto & Caselli 2008, 2010; Keto, Rawlings & Caselli, 2014), while one of the collaborators is leading effort in the ionisation structure of discs (e.g. Ivlev et al. 2016).

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The reduced chemical network will be benchmarked against comprehensive chemical networks to make sure that the abundances of important (diagnostic) species such as C^+, C, O, CO are well reproduced in the range of conditions appropriate for evolved and transitions discs. This will imply running the comprehensive and reduced networks in a grid of physical conditions by varying temperature, density, and UV/X-ray fluxes. As lines of Ne ([NeII], [NeIII]) and Ar ([ArII]) are good tracers of disc winds (e.g. Pascucci 2007, Szulágyi et al. 2012), Ne and Ar will be included in the chemical code.

Particular attention will be dedicated to the inclusion of X-rays and the identification of the regions within the disc where X-rays, FUV photons and cosmic-rays (CRs) dominate the chemical and thermal properties. Typical assumption is that the X-ray spectrum is given by the bremsstrahlung spectrum ($I_\nu \simeq 1/E \times exp(-E/kT)$ on the 0.1 - 10 keV energy range; see Glassgold et al. 2007, Aresu et al. 2011, Meijerink et al. 2012). The observed luminosity ranges are $L_X = 10^{29} - 10^{31}$ erg/s (based on the Taurus survey, Güdel et al. 2007). The X-rays heat up the gas with 10-40% efficiency (UV heating has only a few per cent efficiency).

Impinging X-rays may ionise the disk or wind material via primary or secondary ionisation. Primary ionisation may produce a single or multiple electrons due to the Auger effect. Their energy range depends on from which shell the Auger electron originates. The rate coefficient is given by the integral of the product of the X-ray energy spectrum and the ionisation cross section of the element (see e.g. Meijerink 2012, equation A.13). Secondary electrons might have keV energies, capable of ~20-30 hydrogen ionisation. In fact the secondary electron ionisation rate per H nucleus is higher than the primary by an order of a magnitude, thus often only the secondary ionisations are considered in chemical models (e.g. Ádámkovics et al. 2011, Bruderer 2012). The exact expressions and the peak electronic ionisation cross sections are given in Ádámkovics et al. (2011).

Chemical models in the literature deal differently with X-ray reactions. The Semenov et al. (2010) and associated papers (Akimkin et al. 2013) model these reactions as an additional contribution to cosmic ray ionisation reactions (i.e. the rate is given by $R = \alpha \times (\zeta_{CR} + \zeta_X)$). Bruderer et al. (2012) accounts for only the secondary ionisation. Finally, Meijerink et al. (2012) takes both the primary and secondary ionisation into account, as described above (see also Table 3 in Henning & Semenov 2013).

X-rays affects the chemistry in various ways: (i) X-rays might directly ionise H (while FUV radiation does not), initiating H_2 formation via the H-path. In high temperature regions, where the grain surface H_2 formation is less efficient, this reaction might contribute significantly to the total H_2 formation rate. (ii) Secondary electrons interacting with H_2 produce H_2^+ that quickly react with a further H_2 to form H_3^+ or reforms H_2 via charge transfer with neutral H. This can lead to H_3^+ abundances as high as 10^{-8}. This then initiates efficient ion-neutral reactions which e.g. result in efficient H_2O production (see e.g. Meijerink et al. 2012). Furthermore, the heating effect might also increase the rate of neutral-neutral reactions with reaction barriers. (iii) H_3^+ initiates ion-molecular reactions which keep molecular abundances high even at high temperatures (if X-rays are present, compares to only FUV). (iv) Ne, Ne+, Ar and Ar+ have ionisation potentials 21.56, 40.96, 15.76 and 27.63 eV respectively. They are only ionised due to X-rays or X-ray induced fast electrons. Therefore, their ionisation is an indicator for X-rays and, as already mentioned, these species will be included in our chemical models. (v) Enhanced CO destruction through reaction with He^+, which has an ionisation energy of 24.6 eV (CRs can also ionize it). (vi) Other observational tracers (suggested by Meijerink 2012) are: H_2O, Ne^+, C/C^+ ratio, O^+.

2. **Inclusion of chemistry in dynamical model and radiative tranfer.** Once the reduced network is benchmarked and tested, it will be included in the MOCASSIN-KROME code in collaboration with the postdoc employed on project B2. Radiative transfer codes available at the PI Institute

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(RADMC-3D[2] and LIME[3]) will be used to obtain fluxes in dust continuum and lines to then perform simulated observations and compare with available data and/or make predictions for future observations.

In this second part of the project, we will also explore the effect of varying initial conditions, taking into account effects of accretion, vertical mixing and magnetic disk wind on chemistry following prescriptions by Heinzeller et al. (2011). Often low metal elemental abundances are assumed (H_2 molecular, C^+ ionised) or the chemical network is initially evolved to simulate the conditions of the parent cloud. Depending on what kind of disk wind model is considered, the wind starts to dominate the mass loss rate at different times. For example, EUV winds tend to be efficient at late times, thus the initial chemical composition might not matter, while the X-ray winds might dominate the mass loss over accretion in early times, and thus the initial chemical abundances might matter (see review of Alexander et al. 2014, page 483 end of section 2.3). Furthermore, several papers shows that the radial movement of material and the vertical mixing affect the chemistry in disks, i.e. by lowering concentration gradients and enhancing abundances of NH_3, CH_3OH, C_2H_2 and sulphur-containing species (e.g. Ilger et al. 2004, Semenov et al. 2010, Heinzeller et al. 2011). If the chemical timescales are long compared to the disk wind dynamic time, then the disk composition will affect the wind as well. Thus, we will model the effects of the radial accretion flow and vertical mixing (although the later is more important, see Semenov 2010) on the disk chemistry (even if these motions are not included in the original simulation). As the MOCASSIN simulations start from an alpha-disk model, we will take this disc structure to model the vertical mixing and accretion similarly as was done in the Heinzeller et al. (2011) paper.

3. **Dust evolution.** The chemical model assumes initially that dust grains can be approximated by one-size particles of 0.1μm in diameter and that the dust-to-gas mass ratio is fixed. However, this assumption is completely inappropriate for disc winds. Indeed as explained in detail in project C2 of this proposal, the maximum grain size that can be entrained in the wind at a given radial distance from the star results from the local force balance between the drag force, gravity and the centrifugal force. A further complication is that the underlying distribution of grains is also not constant and varies as a function of disc radius and vertical distance from the mid-plane, due to the effects of grain growth, fragmentation, settling and drift. A detailed model of the spatially and time-varying grain abundances and size distributions in the wind is however essential for the chemical model, since grains provide the bulk of the opacity in the FUV. The third task of the Postdoc employed for this project will be to include spatially-varying grain abundances and size distributions provided by project C2 into the chemical code, at different evolutionary times, to properly account for dust opacities in the wind. Also the effects of different dust grain properties on the chemical composition will be explored at this point. At MPE, we are already studying the effect of varying grain-size distribution on the ionisation structure of discs (Ivlev et al. 2016).

This step will be further decomposed into levels of increasing complexity. We will begin with decoupling the time and space evolution of the grains. We will then compare the timescales involved and asses whether the time-evolution of the dust must be treated self-consistently or if we can work with snapshots.

4. **Time-dependent chemistry.** It is unclear at this stage if equilibrium chemistry is an appropriate approximation for disc winds. The material flows at a few km/sec and as it moves along the wind streamlines it is subject to changes in density and radiation field. It is likely that time dependent calculations will be necessary for this problem, where the dust properties in the chemical code will be provided by the time-dependent calculation of the dust evolution described in C1. This will be the final task of the Postdoc employed for this project, who will first study the time scales

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[2]http://www.ita.uni-heidelberg.de/ dullemond/software/radmc-3d/
[3]http://www.nbi.dk/ brinch/index.php?page=lime

of the various physical/chemical processes (e.g. photochemistry, accretion, mixing, wind) and quantify the validity of equilibrium chemistry.

After this, the whole team will work together to couple time-dependent gas-grain chemistry and dust evolution. Depending on the level of complexity required part of this final step may be carried out in the second funding period.

A Postdoc with at least some experience of astrochemistry would be certainly desirable to work on this complex project. The Postdoc will receive scientific support form the PI, but also from experienced astrochemists and plasma physicists (e.g. Dr Ivlev, Dr Thi and Dr Szücs) at the Centre for Astrochemical Studies led by Prof. Caselli at the MPE.

The final science product will be for the first time a detailed chemical study of a disc wind for one standard case. The lessons learnt will be streamlined and approximated in order to be usable in the parameter space calculations planned for project B1.

2.3 Work programme including proposed research methods

The Gannt chart below describes the time-line of the B2 project:

TASK NAME	Year 1	Year 2	Year 3
The reduced network	- update chemical model - include detailed ionisation processes - insert X-ray chemistry - finalise reduced network		
Chemistry in dynamical model and radiative transfer		- inclusion of chemical code in MOCASSIN by B1 - radiative transfer - comparison with observations	
Dust evolution		- from mono-disperse to grain-size distribution - grain-size from C2	
Time-Dependent chemistry			- study of time scales of various processes - benchmark of time-dependent chemical code - inclusion of time-dependent chemistry in dynamical model

Figure 1: Gannt chart for B2. More details have been outlined in the previous section.

Year 1: (i) focus on the chemical network update, to make sure that all the most recent reaction rates will be included. This will be done by comparing our code with KIDA[4] as well as with comprehensive literature research. (ii) Include detailed ionisation processes, taking into account the effects of

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[4]http://kida.obs.u-bordeaux1.fr

ionisation-recombination from FUV and CRs. (iii) Include X-ray chemistry based on the extensive literature work available as well work done within the ProDiMo code. (iv) Finalise the reduced chemical network, including Ne and Ar, and test/benchmark it.

Year 2: (i) inclusion of reduced chemical network in MOCASSIN-KROME with the help of the B1 team. (ii) The B1 team will then provide the chemical-physical output, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. (iii) Comparison with observations and further update of chemical code based on observational constraints. (iv) Study of the effect of changing the grain size from mono-disperse (0.1 μm) to MRN grain-size distribution (Mathis et al. 1977) or evolved-MRN distributions (e.g. Zhao et al. 2016; Ivlev et al. 2016).

Year 3: (i) study of time scales of various processes in chemical and dynamical model. (ii) Benchmark of time-dependent reduced chemical code. (iii) Inclusion of time-dependent chemistry in dynamical model.

2.4 Data handling

Discuss on how the results will be 'packaged' to be used by other sub-projects as well as from the community. e.g. Could the network be made public? or the research unit website? what other products could be interesting to the community outside our research unit?

2.5 Other information

[Text]

2.6 Information on scientific and financial involvement of international cooperation partners

[Text]

3. Bibliography

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

[Text]

4.1.2 Direct Project Costs

[Text]

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

[Text]

4.1.2.2 Travel Expenses

[Text]

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

[Text]

4.1.2.4 Other Costs

[Text]

4.1.2.5 Project-related publication expenses

[Text]

4.1.3 Instrumentation

[Text]

4.1.3.1 Equipment exceeding EUR 10,000

[Text]

4.1.3.2 Major Instrumentation exceeding EUR 100,000

[Text]

4.2 Module Temporary Position

[Text]

4.3 Module Replacement Funding

[Text]

4.4 Module Mercator Fellows

[Text]

4.5 Module Public Relations Funding

[Text]

5. Project requirements

5.1 Employment status information

[Text]

5.2 First-time proposal data

[Text]

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5.3 Composition of the project group

[Text]

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

[Text]

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

[Text]

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

[Text]

5.5 Scientific equipment

[Text]

5.6 Project-relevant interests in commercial enterprises

[Text]

5.7 Additional information

[Text]