Cover sheet to application

1 Personal data application

Name, first name	Lic. Kevin Speyer
subject area	Physics
personal ID	91703661
University	Universität Göttingen
offer country	Argentina
Scholarship programme	Research Grants - Short-Term Grants, 2018
Scholarship period	May 1, 2018 to Jul 1, 2018
Resp. DAAD Unit	ST31 Lateinamerika

2 Documents for application

which you upload your application documents are listed below.

Type of document	Name of the document
Curriculum vitae	CV_Kevin_Speyer.pdf
List of publications	List_of_Publications.pdf
Study project/motivation	Research_Proposal.pdf
Time schedule	Schedule_of_Work.pdf
Contacts at host institution	Invitation_Letter.pdf
University degree certificates	MS_degree_Spanish.pdf
University degree certificates	MS_degree_English.pdf
Transcript of records/academic achievements	Transcript_Spanish.pdf
Transcript of records/academic achievements	Transcript_English.pdf
Proof of admissionProof of admission	Scholarship_PhD_Certificate_Spanish.pdf
Proof of admissionProof of admission	Scholarship_Certificate_English.pdf

Application

1 General information

Scholarship programme	Research Grants - Short-Term Grants, 2018
Status	Doctoral candidate

2 Details for application

Note on completing the application form:

* Compulsory field (must be completed).

(*)Dependant compulsory field (must be completed if at least one other field in this section is completed).

1

Family name *	Speyer				
if applicable, name at birth					
Academic title	Lic.				
First name(s) *	Kevin				
Date of birth *	11.05.1987	Place of birth *	Buenos Aires	Country of birth*	Argentina
Nationality *	Argentine	2. Nationality	German		
Form of address *	Mr.	Marital status *	partnership		
Number of children	0				

2

Country of permanent residence from where you are applying for a scholarship/funding *

Argentina

Is your country of origin different from the country in which you live permanently? * yes ○ no ◉

If yes, which? * Select country

2 Details for application

3 Home address

(Address at which you can be contacted currently)

c/o name	
street address or PO box *	Gutenberg 240
Zip code	1427
City *	CABA
Country *	Argentina
Telephone number	
Mobile phone number	005491162089696
Fax	
Email address *	speyer.kevin@gmail.com

Only use these fields to enter additional address information that find no place in the standard mandatory address details above.

2 Details for application

4 Name and address of next of kin who should be contacted in an emergency.

yes (●) no ( )

Name	Speyer
First name	Diego
Additional address information 1	Ballivian 3283, CABA, Argentina
Additional address information 2	
c/o name	
street address or PO box	Ballivian 3283
Zip code	1431
City	CABA
Country	Argentina
Telephone number	
Mobile phone	+5491150138890
Fax	
Email address	dspeyer@chbsym.com.ar

5

2 Details for application

Please enter your destination institution / university

Planned destination institution 1 *

Destination country * Germany City * Göttingen

Institution * Universität Göttingen

Other institution ☐

Subject group * Math / Science

Subject * Physics

Planned destination institution 2 alternatively ○ additionally ○ None ◉

6 Subject area / discipline / research field the application refers to

Subject group * Math / Science

Subject * Physics

Explanation

7 What made you choose your host institution/host university? * My PhD Supervisor, Dr. Claudio Pastorino, has collaborated in several projects with Prof. Dr. Marcus Müller over the years. Dr. Marcus Müller works in the University of Göttingen. The University own very advanced equipment to successfully perform the planned research activities.

Is your stay part of a cooperation agreement? *

yes ◉ none ○

8 Do you already have contacts there? * yes ◉ none ○

With Whom? Prof. Dr. Marcus Müller

2 Details for application

9 Do you have confirmation that you have academic supervision?*

yes ◉ none ○

Have you received notification that you satisfy admission requirements? *

yes ◉ no ○

10 Planned duration of stay: from 01.05.2018 to 01.07.2018

11 Duration of requested funding: from * 01.05.2018 to * 01.07.2018

12 Short description of research/study/work project *(An extensive description should be added on a separate sheet)

Using large-scale computer simulation of coarse-grained polymer models we propose the study of the non-equilibrium self-organization of active polymer brushes in response to a periodic driving. We will analyze the intricate interplay between the non-equilibrium single-chain dynamics , the collective behavior of the interacting brush chains, and the liquid flow past the brush-coated surface.

13 Secondary school *

Type of qualification * Bachelor in Science and Arts

Date * 02.12.2004 City / Province * Buenos Aires

Result * 7.2 out of 10

Length of school attendance

from * 01.03.1999 to * 02.12.2004

14 Completed examinations (if applicable) (*)

2 Details for application

Entry 1

Institution	University of Buenos Aires		
Period: from	03.04.2006	to	28.03.2014
Subject group	Math / Science		
Subject	Physics		
Type of exam	Master's degree (or equivalent)		
Result	9.26 / 10		

new entry | Delete this entry

15 Current/last home Institution

Institution *	CONICET	
Type study programme *	Doctarate	
Major *	Subject group *	Math / Science
	Subject *	Physics
2nd subject	Subject group	Select group...
	Subject	(Please select first group of subjects.)
3rd subject	Subject group	Select group...
	Subject	(Please select first group of subjects.)

2 Details for application

16 What will be your highest academic qualification at the time your scholarship begins?

Will you have a degree when your funding begins? yes ◉ no ○

Qualification *	Master's degree (or equivalent)
(Planned) date of completion *	28.3.2014
Name *	Licentiate in Physical Sciences
Subject group *	Math / Science
Subject *	Physics

17 Previous study/research/working stays or other activities abroad

Entry 1

Country	Italy		
Institution, City/Province	ICTP, Trieste		
Period: from	03.10.2016	to	14.10.2016
Purpose	Participate in a Workshop		

new entry | Delete this entry

Entry 2

Country	Italy		
Institution, City/Province	ICTP, Tireste		
Period: from	07.03.2016	to	18.03.2016
Purpose	Participate in a Workshop		

new entry | Delete this entry

2 Details for application

Entry 3

Country	Germany		
Institution, City/Province	Ludwig-Thoma-Gymnasium, Bayern		
Period: from	01.12.2003	to	29.02.2004
Purpose	High school student exchange		

new entry | Delete this entry

18 Previous and current professional / teaching or artistic activities.

Entry 1

Institution, City / Province	San Martín University, Buenos Aires		
Period: from	03.08.2015	to	22.12.2015
Activity	Teaching Assistant		

new entry | Delete this entry

Entry 2

Institution, City / Province	University of Buenos Aires		
Period: from	01.03.2013	to	20.12.2014
Activity	Teaching Assistant		

new entry | Delete this entry

Entry 3

Institution, City / Province	University of Buenos Aires (CBC)		
Period: from	01.03.2012	to	20.12.2013
Activity	Teaching Assistant		

new entry | Delete this entry

2 Details for application

19 Previous and current scholarships from the DAAD or other organisations *

yes ◉ none ○

Funding organisation / programme *	from *	to *
ICTP	03.10.2016	14.10.2016
ICTP	07.03.2016	18.03.2016
CONICET, Full PhD Scholarship	01.04.2014	31.03.2019

20 Do you aim to obtain a degree? * yes ◉ no ○

What kind of degree do you aim to obtain? * Doctorate/Ph.D (or equivalent)

Double degree * yes ○ no ◉

Where do you intend to obtain your degree? *

- Home university ☒
- Destination university ☐
- Other university/institution ☐

Do you intend gaining the degree during the scholarship period? * yes ○ None ◉

2 Details for application

21 Will you receive a salary, annuity, grant or similar from an employer or public institution during the funding period for which you are applying?*

yes ◉ no ○ planned ○

(If yes, please state the type of payment:)

If yes, please state the type of payment	CONICET
Total monthly payment	18.981,24
Payment *	Argentinian Austral

22 Will you be funded by another organisation during the planned funding period or have you applied for other funding for this period? *

yes ○ no ◉

From which?

Organisation *	Status	from *	to *
	Select status...		
	Select status...		
	Select status...		

23

Documented language skills

Language	German
Certificate	Deutsches Sprachdiplom Stufe II der Kultusministerkonferenz
Grade/points	78

2. Add language | 2. remove language

2 Details for application

Language 2: English

Certificate: PET

Grade/points: PASS

3. Add language | 3. remove language

Description of other language(s):

24 Language skills (not documented)

Language	very good	good	average	poor
Spanish	●	○	○	○
English_GB	●	○	○	○
Portuguese	○	○	●	○

Description of other language(s):

25 What other extracurricular activities/interests would you like to mention?

As a hobby I like to implement my programm experience to create Home Automation gadgets with microcontrollers and sensors. For example, I have assemble an intelligent watering system for plants, with an Arduino, a soil humidity sensor a relay and an electrovalve.

26 Professional goal

2 Details for application

27

Other comments/information you think might be of relevance to your application or which should be included in the assessment of your achievements and personal suitability
(e.g. details about special extracurricular activities, but also impediments such as illness or disability, if this had a negative impact on your academic progress/achievements and should be considered in a comparison of applicants).

Important notice

Please save the form after editing on your computer. Please use the „save as" option to be aware of the file location of the last edited version of the application form on your computer. You can return to the portal to upload the edited form and continue your application by clicking the link

DAAD-Portal öffnen

Kevin Speyer – Curriculum Vitae

Address	Gutenberg 240, Buenos Aires City, Argentina
Date of Birth	11^{th} May 1987
Nationality	Argentinian / German
Mobile Phone	+54 9 11 6208 9696
Email	speyer.kevin@gmail.com

Current Position

PhD candidate in Physics

Thesis	Simulations of liquid flow confined by semiflexible polymer brushes
University	University of Buenos Aires, Argentina
Workplace	National Atomic Energy Commission (CNEA)
Scholarship	2014 - 2019 by the National Scientific and Technical Research Council (CONICET)
Supervisor	Dr. Claudio Pastorino

Education

2014-Present	PhD Candidate in physics by the University of Buenos Aires with a scholarship of the National Scientific and Technical Research Council (CONICET)
2006-2014	Diploma in Physics (M.S. equivalent) by the University of Buenos Aires (Avg: 9.26 / 10)
1999-2004	High school Pestalozzi
2004	Sprachdiplom Stufe II, German Language Certificate of the Education Ministers Conference
12/2003-3/2004	Student Exchange in Germany, attending classes and staying with a German host family
2002	Sprachdiplom I, German Language Certificate of the Education Ministers Conference
2001	Preliminary English Test, Cambridge University

Scholarships and Internship

10/2016 & 3/2016	International Centre for Theoretical Physics to participate in Workshops
3/2014 - 3/2019	National Scientific and Technical Research Council (CONICET), full scholarship for PhD studies
12/2004	Bayer, paid internship

Conferences

9/2017	102th National Reunion of the Argentine Physics Association
11/2016	Frontiers in Physical Science, Max Planck, Argentina
10/2016	Introductory School on Parallel Programming and Parallel Architecture for High-Performance Computing, ICTP, Italy
3/2016	4th Workshop on Advanced Techniques for Scientific Programming and Management of Open source Software Packages, ICTP, Italy
9/2015	100th National Reunion of the Argentine Physics Association
6/2015	4th International Workshop "Theory and Computer Simulation of Polymers: New Developments, Germany
3/2015	Workshop: Dynamics in Soft and Hard Condensed Matter, Argentina
11/2014	First Argentinian Microfludics Workshop
9/2014	5th Argentinian Soft Matter Encounter
9/2014	99th National Reunion of the Argentine Physics Association

Languages

Spanish	Native
English	Fluent
German	Fluent
Portuguese	Basic

Programming Skills

Advanced in	Linux environment, Python, C++, Fortran, LabView, awk, Matlab and git

Teaching and Work Experience

8/2015 12/2015	Teaching Assistant at the Sto institute of the San Martational University for Introduction to Computer Simulation
3/2013 12/2014	Teaching Assitant at the physics department from the University of Buenos Aires for Physics I for Biologists and Physics II for Biologists
3/2012 - 12/2013	Teaching Assistant at the Common Basic Cycle (Foundation Year equiv.) at the University of Buenos Aires for Physics and Introduction to Biophysics
2/12/04 - 31/12/04	Internship at Bayer S.A. in the Trade Marketing area, Bayer Health Care (BHC) performing administrative tasks

Scientific Publications

- Brushes of semiflexible polymers in equilibrium and under flow in super-hydrophobic regime
K. Speyer and C. Pastorino, Soft Matter, 2015, 11, 54735484
DOI:10.1039/C5SM01075F

- Droplet transport in a nanochannel coated by hydrophobic semiflexible polymer brushes: the effect of chain stiffness
K. Speyer and C. Pastorino, Langmuir, 2017, 33 , 1075310763
DOI:10.1021/acs.langmuir.7b02640

Interests and Skills

- Polymer Physics, Soft Matter and Microfluidics
- Atomistic and coarse grain high performance computer simulations
- Statistical Analysis of Big Data
- Experience with Laboratory Equipment and single-board microcontrollers such as and Arduino Raspberry Pi

List Of Publications

- Brushes of semiflexible polymers in equilibrium and under flow in a super-hydrophobic regime
  K. Speyer and C. Pastorino, *Soft Matter*, 2015, **11**, 5473–5484
  DOI:10.1039/C5SM01075F

- Droplet transport in a nanochannel coated by hydrophobic semiflexible polymer brushes: the effect of chain stiffness
  K. Speyer and C. Pastorino, *Langmuir*, 2017, **33** , 10753–10763
  DOI:10.1021/acs.langmuir.7b02640

DAAD Short-term grant application
Active polymer brushes

December 1, 2017

Applicant:	Lic. Kevin Speyer
Home institution:	National Atomic Energy Commission, Pcia. Buenos Aires, Argentina
Host institution:	Institut für Theoretische Physik, Georg-August Universität, Göttingen
Duration:	2 months
Starting date:	May 2018

1 Introduction

Polymers are long, (semi)flexible macromolecules that are comprised of a sequence of monomeric repeating units that are joined into a linear chain molecule. These linear polymers are ubiquitous, both in form of synthetic materials as well as in biological systems. Irreversible grafting polymers with one chain end onto a solid substrate is a versatile strategy to tailor surface properties such as adhesion, wettability, friction, as well as optical or electronic properties. In contrast to coatings that rely on physical adsorption, polymer brushes formed by grafting polymers to or from surfaces are significantly more stable against mechanical load or chemical exposure [1]. Therefore, brush-coated surfaces have found ample applications, ranging from colloidal stabilization of paints and coatings of textiles to lubricating layers in human joints.

Additionally, polymer brushes are able to respond to various environmental stimuli. For instance, multi-component brushes can exhibit hydrophilic or hydrophobic surface properties, form lateral structures, or switch between protein-resistant and protein-adsorbing states [2]. The stimuli can consist of thermodynamic control parameters like pH-value or temperature of the surrounding solvent, or external electric or magnetic fields. Much effort has been focused on quasi-static fields that are switched once, and subsequently, the system relaxes into a new equilibrium state. A notable exception is the transport of nanoparticles on polymer brushes by periodic exposure to different solvents [3]. In this case, however, the time period is still much larger than the molecular time scale. Much less is known, however, if the time scale of the external stimulus is comparable to the relaxation time of the polymers themselves.

During the research visit of Kevin Speyer at the Institute for Theoretical Physics at the Georg-August University in Göttingen, we will explore the self-organization of polymer

brushes subjected to periodic external stimuli. The time period of the external stimuli will overlap with the spectrum of relaxation times of the semiflexible grafted polymers. This challenging project builds upon the sophisticated simulation techniques that Kevin Speyer has learned to master in the course of his successful Ph.D. project at the National Atomic Energy Commission in Argentina, and it extends his previous studies towards a new research area.

The project description is arranged as follows: The next section provides a report on the achievements that Kevin Speyer has already achieved in his Ph.D project. Further details can be found in the two pertinent publications in Soft Matter and Langmuir. The following section, presents the goals and methods of the new project. A detailed work plan is compiled in the concluding section.

2 Kevin Speyer's previous research work

Already during his Diploma Thesis (MS equivalent), entitled "Simulation of simple liquids confined in soft channels", the candidate – Kevin Speyer – studied a nanochannel with confining surfaces coated with grafted polymers. In this work, the interaction between the liquid and the grafted polymers was analyzed in equilibrium and in flow conditions. This first study focused on the influence of the bending rigidity of semiflexible polymers on the static and dynamical properties of the system. The soft brush substrate is hydrophobic, i.e., there is a repulsion between the brush polymers and the solvent, giving rise to a Cassie–Baxter state. In this state, the liquid does not contact the grafting surface but is suspended by the polymer brush on void pockets. Equilibrium properties such as brush height and bending energy were measured, varying the grafting density (number of chains per surface area) and the stiffness of the polymers. The characteristics of the brush–liquid interface and the morphology of the polymer chains supporting the liquid were studied for different bending rigidities.

Non-equilibrium simulations were performed, moving the walls of the channel in opposite directions at constant speed, obtaining a Couette velocity profile in the bulk liquid. The molecular degrees of freedom of the polymers were investigated as a function of the shear rate. The violation of the no-slip boundary condition and the slip properties were analyzed as a function of the shear rate, grafting density and bending stiffness. At high grafting densities a finite slip-length, independent of the shear rate or bending constant, was found, whereas at low grafting densities a very interesting non-monotonic dependence on the bending constant was observed. This work was published in the international peer-reviewed journal *Soft Matter* [4].

During his Ph.D project that is sponsored by a Ph.D CONICET scholarship, Kevin Speyer analyzed a system composed of a liquid droplet in a slit-like nanochannel, coated with semiflexible hydrophobic polymers by means of non-equilibrium molecular dynamics simulations. This work is performed in the group "Theory and Simulation of Soft Matter", headed by Claudio Pastorino at National Atomic Energy Commission (CAC-CNEA) in Argentina. The polymer chains, grafted by an terminal bead to the confining walls, are described by a coarse-grained, bead-spring model that accounts for chain connectivity,

excluded volume interactions and local chain stiffness. The liquid droplet is confined by brush-coated surfaces and coexists with its vapor phase. In response to an external body force (aka pressure difference), the droplet moves. The rheological, frictional and dynamical properties of the brush were studied over a wide range of persistence lengths, and a rich behavior of polymer conformations and concomitant changes in the friction properties were found over the wide range of studied polymer stiffness. A rapid decrease in the droplet velocity was observed as the rigidity of the chains is increased for polymers whose persistence length is smaller than their contour length. A strong correlation between the internal dynamics of the brush and the droplet-transport properties was found, which could be used to tailor flow properties by surface functionalization. The monomers of the brush layer, under the droplet, present a collective "treadmill belt" like dynamics, which highlights the existence of grafted chains. The changes in spatial extension upon variations of polymer stiffness were quantified by two-dimensional velocity and density profiles. The deformation of the polymer brushes due to the presence of the droplet has been analyzed in detail. Lastly, the droplet−vapor interaction has been studied by varying the liquid–to–vapor ratio, observing an increase of droplet speed for a small spatial separation of droplets, compared to a train of droplets that present a large gap between consecutive droplets. These results were recently published in *Langmuir* [5].

Kevin Speyer works on a daily basis on large computer clusters, running coarse-grained simulations and performing post-processing statistical analysis with scripting languages (python, awk). He is familiar with various visualization tools for 3D atom dynamics (Visual Molecular Dynamics), color plots and data visualization (python, Xmgrace, gnuplot) and has experience in High Performance Computing, including parallelization techniques with MPI.

To summarize, the candidate – Kevin Speyer – brings to the project significant experience in molecular dynamics simulation of semiflexible polymer brushes in equilibrium and under externally driven, stationary flow. He is acquainted with parallel molecular dynamics simulation of coarse-grained models of polymers, and his research in his master and Ph.D thesis has already resulted in two publications in renown international scientific journals. The coarse-grained representation and simulation techniques will also be employed in the proposed project. These ideal qualifications of the candidate ensure that the new project on "active polymer brushes" will have a flying start in terms of techniques, yet it will explore a fundamentally new aspect of the dynamical behavior of polymer brushes.

3 Project: Active polymer brushes

Using large-scale computer simulation of coarse-grained polymer models we propose the study of the non-equilibrium self-organization of active polymer brushes in response to a periodic driving. We expect an intricate interplay between the non-equilibrium single-chain dynamics ("tumbling motion"), the collective behavior of the interacting brush chains, and the liquid flow past the brush-coated surface. Our simulation study will elucidate to what extent the individual molecular motions are coupled and synchronized (spatiotemporal correlations), what dynamic structures arise in the polymer brush, and how the collective

brush dynamics impacts the transport of liquid or adsorbing solutes, as well as the friction of the liquid slipping past the externally driven surface. We expect that the external energy input and dissipation in the polymer brush gives rise to a rich dynamical behavior (e.g., oscillatory response of the brush) as a function of the properties of the polymer brush (grafting density and stiffness) and the liquid, and the matching of the external driving frequency with the spectrum of relaxation times of the brush.

This project nicely fits in the overarching topic of Kevin Speyer's Ph.D thesis and will provide him with the opportunity to learn about modern concepts of non-equilibrium statistical mechanics and state-of-the-art simulation techniques on clusters of CPUs and GPUs at German supercomputer centers (GWDG Göttingen, HLRN Hannover/Berlin, and NIC, Jülich). The topic of the project also strengthens the longstanding collaboration between the home institution (group of Claudio Pastorino) and the host institution (group of Marcus Müller), utilizing coarse-grained computer simulations to study polymer brushes under flow [6, 7, 8, 9], exploring how the brush coating dictates the hydrodynamic boundary condition [10, 11], and investigating the tumbling motion of the individual grafted macromolecules and the concomitant reversal of the near-surface flow under shear [12, 13].

3.1 Goal

The goal of Kevin Speyer's project – active polymer brushes – consists in using molecular dynamics simulation of coarse-grained models to design the response of polymer brushes to periodic external driving forces so that the external energy input gives rise to a collective dynamics that enhances transport of fluid or adsorbed solutes at the brush-liquid interface.

The coating of the surfaces with tethered polymers alters the flow properties in the ultimate vicinity of the brush-covered surface. These boundary effects become particular important in microfluidic devices that manipulate confined liquids at the pico-liter scale, electroosmotic flow, or vascular biological systems [14]. Much interest has focused on driving the liquid motion externally, e.g., by a pressure difference, shear of confining boundaries, or an external, electric field. Such conditions are particularly relevant for applications such as lab-on-chip devices [15, 16], controlled drug delivery, functionalized surfaces and sensing at the nano-scale. However, all these external driving forces are quasi-static, i.e., their characteristic time scale is infinite in comparison to the spectrum of molecular relaxation times.

Active particles and polymers in biological context or synthetic realizations constitute an alternative driving mechanism that has attracted much attention recently. In these systems, the active entities possess internal degrees of freedom that enable them to take energy from the environment and perform mechanical work in the form of, e.g., systematic movements. Active systems under study range from bacteria [17] or spermatozoa, to smaller functional units of cells and micro-organisms such as cilia, flagella and molecular motors [18, 19]. These last cases include also so-called micro-swimmers of biological origin, such as opalinas and chlamydomonas or synthetic experimental systems such as self-propelled droplets, catalytic Janus colloids or thermophoretic nano-particles [19]. Understanding the mechanisms how the coupling among active units results in directional motion [20, 21, 22, 23, 24] and the collective states of these active materials is of great current interest.

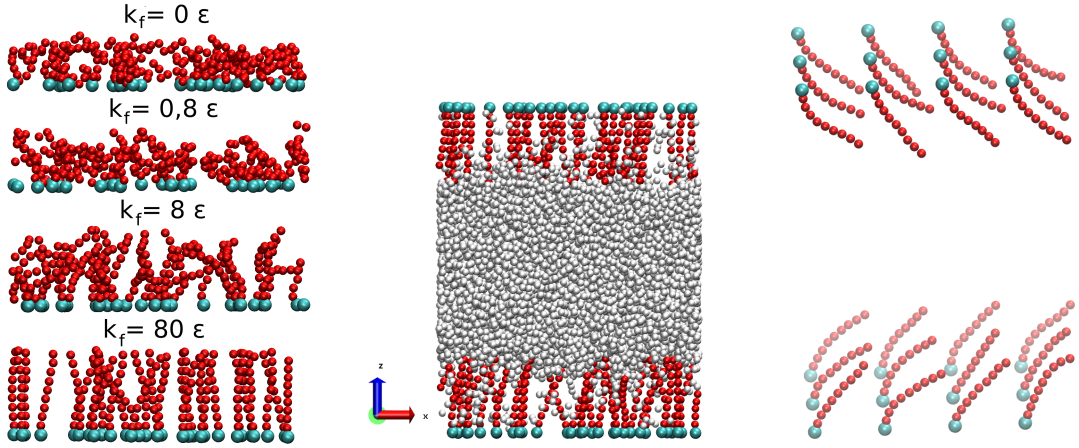

Figure 1: Left panel: Grafted polymer layers with increasing stiffness, which is parameterized by the bending constant k_f. Center panel: Planar channel filled with liquid confined between two stiff polymer brush layers with $k_f = 80$. Right panel: Illustration of an active brush oscillating with the same phase (phase-locked state, grafting points arranged on square lattice).

The coordinated motion of cilia, which are comprised of active, semiflexible filaments anchored to a surface, can give rise to directed motion of micro-organisms in nature or to pumping of fluids in certain tissues. For example, cilia in the human respiratory tract pump viscous fluids away from the lungs or propel dust particles out of the body. This amazing function and the efficiency of cilia transport has stimulated research groups to design synthetic analogues in order to regulate flow or particle motion in microfluidic devices.

We propose to study planar nano-channels coated by active polymers, end-grafted to the confining walls of a narrow slit channel. In this short-term project we do not focus on modeling the intricate internal mechanism that drives the autonomous motion of biological cilia but we rather investigate the self-organization of externally driven polymer brushes. This strategy allows us to systematically explore different driving mechanism that are inspired by the prototypical motion of cilia or flagellae, and we will optimize the external driving of semi-flexible polymer brushes to result in a efficient, collective, directed near-surface transport.

A preliminary feasibility study that illustrates this kind of driving in our coarse-grained model of semiflexible brushes is presented in Fig. 1. The asymmetric beating pattern of the semiflexible polymers consists of a power stroke and a recovery stroke – essential features of active, biological systems. In the former the cilium stretches out and moves rather fast in one direction. In the recovery stroke, in turn, the cilium bends and slowly retracts [19].

This asymmetric motion results from an internal activity in biological cilia. In our project is driven by an external, periodic force that acts on the bottom part of the grafted polymers. As a first step, we have begun to characterize the polymer motion in the absence of an explicit solvent, where there is no hydrodynamic coupling between grafted molecules. Neighboring brush molecules are only coupled via the direct steric interaction (i.e., chain molecules cannot cross through each other in the course of their motion) or, additionally,

via a harmonic coupling of neighboring chains close to the grafting point. This very simple model already exhibits different behaviors as a function of the frequency of the driving forces, and details of the coupling between neighboring chains. Based on these promising results, we will immerse the brush in a simple liquid and study the collective dynamics and synchronization as well as the impact of the driving on the dynamics of the liquid.

During his two-month stay in Göttingen, Kevin Speyer will address the following specific questions:

- What is the relative importance of mechanical/steric and hydrodynamic interactions in the collective dynamics and synchronization of the polymer chains?
- How can one optimize the asymmetric motion pattern of the semiflexible grafted polymers to produce a directed flow at the vicinity of the brush-liquid interface?

Having achieved an understanding of these two basic questions there are several extensions that could be pursued in the following, final year of Kevin Speyer's Ph.D. project. The specific selection depends of the outcome of the present project but two follow-up studies illustrate the potential of this new project.

- How does the externally driven motion of the brush coating affect the friction of the brush-coated surface. Can one tailor the friction properties by the external driving or can one impart an anisotropy?
- Methachronal waves are frequently observed in biological cilia, i.e., there are regions of perfect synchronization surrounded by disordered beating patterns. Can one observe similar features in externally driven systems?

3.2 Methodology

In accord with Kevin Speyer's previous work, we will use molecular dynamics simulations of coarse-grained bead-spring models. The active polymer brushes are described by the Kremer-Grest model [25, 26], where segments interact via a Lennard-Jones potential describing the harsh excluded volume of individual segments. A Finite Non-linear Extensively Elastic (FENE) potential accounts for the chain connectivity. We have used this model in our previous joint work on polymer brushes [6, 8, 13]. Additionally, we apply a harmonic bending potential between two consecutive bonds that connect a given monomer with its two nearest neighbors in order to tune the rigidity of the semi-flexible polymer chain [4].

The applicant has significant experience in the study of semi-flexible brushes under flow and has implemented the bending potential in the self-written, MPI-parallel molecular dynamics program [4, 5]. Importantly, the combination of harsh excluded-volume interactions between segments and a maximal bond length guarantees that chain contours cannot cross through each other in the course of the simulation [25, 26]. These entanglement effects that dramatically alter the dynamics in dense melts of long polymers are expected to be important for the synchronization of the active polymers.

We are planning the use of molecular dynamics simulation with a DPD (or Lowe-Anderson) thermostat [27, 28]. This pairwise thermostat obeys translation invariance and

locally conserves momentum, thereby duly accounting for hydrodynamic interactions that are mediated via the explicit solvent [9, 7, 29]. We have experience in using this simulation techniques to study isothermal flows in nano-channels [12, 29, 13, 11].

The MPI-parallel simulation code of the Argentine group is well suited for computer clusters; in Göttingen, the applicant will have additionally the opportunity to learn the use and programming of a GPU-program that is based on the HOOMD code (see http://glotzerlab.engin.umich.edu/hoomd-blue). The latter allows for large-scale simulations on clusters of GPUs that are available at the von-Neumann Institute for Computing (NIC) in Jülich. This transfer of knowledge will be beneficial for the Argentine group because of the availability of computational resources in Göttingen and the very good performance-to-price ratio of GPUs. Additionally, the research stay in Göttingen will offer opportunities to interact with the members of the SFB 937 "Collective behavior of soft and biological matter ", in particular the group of Jörg Enderlein (III Institute of Physics) and Eberhard Bodenschatz (MPI for dynamics and self-organization).

4 Detailed work plan

- Channel with explicit solvent: synchronization and hydrodynamic coupling
  - An explicit solvent will be added to channels coated by active brushes, described by Lennard-Jones particles, to account for momentum conservation and the concomitant hydrodynamic interactions, taking advantage of the experience of the German group.
  - We will analyze the effect of solvent-mediated hydrodynamic coupling between active chains and characterize changes in the collective chain dynamics, as compared to the case of elastic coupling alone (in dry brushes).
- Liquid flow with synchronized chain dynamics
  - Imposing coordinated movement to the chains, mimicking typical cilia dynamics, we will study the flow generated in the solvent.
  - Upper and lower active brush layers of the slit channel will be studied as a function of polymer beating frequency, amplitude, and direction. Directed flow in the vicinity of the individual active brush layers can be achieved by choosing parameters that result in synchronization or by imposing a phase-locked dynamics with a time-dependent external force.
  - Special interesting cases are in-phase movement of active upper and lower brushes and anti-phase movement of upper and lower grafted layers. If the polymers drive locally the fluid, the in-phase movement is expected to produce a plug flow, whereas the anti-phase movement results in shear flow.
  - A parallelization scheme with GPU of some parts of the code will be studied and implemented by the applicant with the help of the Prof. Müller and his group.

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Schedule of planned research work
Active polymer brushes

December 1, 2017

Applicant:	Lic. Kevin Speyer
Home institution:	National Atomic Energy Commission, Pcia. Buenos Aires, Argentina
Host institution:	Institut für Theoretische Physik, Georg-August Universität, Göttingen
Duration:	2 months
Starting date:	May 2018

1 Schedule

- 1 May to 1 June: Channel with explicit solvent: synchronization and hydrodynamic coupling
  - An explicit solvent will be added to channel coated by active brushes, described by Lennard-Jones particles, to account for momentum conservation and the concomitant hydrodynamic interactions, taking advantage of the experience of the German group.
  - We will analyze the effect of solvent-mediated hydrodynamic coupling between active chains and characterize changes in the collective chain dynamics, as compared to the case of elastic coupling alone (in dry brushes).
- 1 June to 1 July: Liquid flow with synchronized chain dynamics
  - Imposing coordinated movement to the chains, mimicking typical cilia dynamics, we will study the flow generated in the solvent.
  - Upper and lower active brush layers of the slit channel will be studied as a function of polymer beating frequency, amplitude, and direction. Directed flow in the vicinity of the individual active brush layers can be achieved by choosing parameters that result in synchronization, or by imposing a phase-locked dynamics with a time-dependent external force.
  - Special interesting cases are in-phase movement of active upper and lower brushes and anti-phase movement of upper and lower grafted layers. If the polymers

drive locally the fluid, the in-phase movement is expected to produce a plug flow, whereas the anti-phase movement results in shear flow.

– A parallelization scheme with GPU of some parts of the code will be studied and implemented by the applicant with the help of the Prof. Müller and his group.

Prof. Dr. M. Müller
Institut für Theoretische Physik,
Friedrich-Hund-Patz 1, D-37077 Göttingen, Germany

GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Mr. Kevin Speyer
Comision Nacional de Energia Atomica (CNEA)
Departamento de Fisica de Materia Condensada
Pcia. Buenos Aires, Argentina

Prof. Dr. Marcus Müller

Telefon: (0551)39-13 88 8
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Fax: (0551)39-9631
E-Mail: glormann@theorie.physik.uni-goettingen.de

Re: Arbeitsplatzzusage für Herrn Kevin Speyer

28. November 2017

Dear Kevin,

I most strongly support your application to the DAAD for a two-month research visit in May-July to my group at the Institute for Theoretical Physics at the Georg-August University, Göttingen. Your stay in Göttingen will provide us with the exciting opportunity to collaborate on the fascinating topic of mutual interest – active polymer brushes – and I envision many fruitful interactions with the members of my group on polymer and soft-matter physics as well as scientific computing as well as researchers in Göttingen, in particular, within the SFB 937 “Collective behavior of Soft and Biological Matter”. We will provide office space, infrastructure (secretarial support, library access, etc), and assist you in searching for accommodation. Moreover, you will obtain access to state-of-the-art supercomputers at the GWDG Göttingen and the Neumann Institute for Computing.

I am looking very forward to hosting you and collaborating with you in Göttingen.
With best wishes

Marcus Müller

(Marcus Müller)

REPÚBLICA ARGENTINA

Universidad de Buenos Aires

Facultad de Ciencias Exactas y Naturales

El Rector de la Universidad y el Decano de la Facultad

Por cuanto, **Kevin Speyer**

natural de la Ciudad de Buenos Aires, ha finalizado el 28 de marzo de 2014 los estudios correspondientes a la **Licenciatura en Ciencias Físicas.**

Por lo tanto, de acuerdo con las normas vigentes en esta Universidad, le confieren el presente diploma de **Licenciado en Ciencias Físicas.**

Buenos Aires, 11 de mayo de 2015

Dr. JUAN CARLOS REBOREDA
DECANO

Dra. INES CAMILLONI
SECRETARIA ACADEMICA

ALBERTO E. BARBIERI
RECTOR

MARÍA CATALINA NOSIGLIA
SECRETARIA DE ASUNTOS ACADEMICOS

Documento Nacional de Identidad 33023577

LEONARDO FEDERICO GOTTIFREDI
DIRECTOR GENERAL DE TITULOS Y PLANES

MINISTERIO DE EDUCACIÓN

DIRECCIÓN NACIONAL DE GESTIÓN UNIVERSITARIA

Certifico que las firmas del Rector, Dr. Alberto Edgardo BARBIERI, Secretaria de Asuntos Académicos, Lic. Maria Catalina NOSIGLIA y el Director General de Títulos y Planes, Sr. Leonardo Federico GOTTIFREDI que anteceden, guardan similitud con la/s que obran en nuestros registros.

Buenos Aires, 17 JUL 2015

Ministerio de Educación
Presidencia de la Nación

ME000000778341

Firma del interesado

REGISTRADO EN EL LIBRO GENENERAL DE GRADOS Nº 226 FOLIO 177 CON EL Nº 5502

Argentine Republic

University of Buenos Aires
Faculty of Exact and Natural Sciences

The Rector of the University and the Dean of the Faculty

Considering that Kevin Speyer born in the city of Buenos Aires, has finalized on the 28th of march of 2014 the studies corresponding to Licentiate* in Physical Sciences.
Therefore, according to the current norms in this University, we confer him the present degree of Licentiate* in Physical Sciences

Buenos Aires, 11th May of 2015

Dr. Ines Camillon	Dr. Juan Carlos Reboreda	Alberto E. Barbieri	Maria Catalina Nosiglia
Academic Secretary	Dean	Rector	Secretary of Academic Affairs

* Translator's Note: The Licentiate Grade is equivalent to a MS degree.

UNIVERSIDAD DE BUENOS AIRES

Facultad de Cs. Exactas y Naturales

Certificado de Materias

El que suscribe certifica que en la foja Nro.:L 184/006 correspondiente al Alumno Sr. SPEYER KEVIN.----------
de la carrera de Cs.Físicas (002) se encuentran registrados los exámenes que a continuación se indican:

A S I G N A T U R A S	CALIFIC.	COND.	ACTA/RE	FECHA
FISICA (03)(CBC)	7 Siete.	Ofic.	R 99999	02/07/05
INT.CONOC.SOCIEDAD Y EL ESTADO (24)(CBC)	8 Ocho.	Ofic.	R 99999	02/07/05
ANALISIS MATEMATICO (28)(CBC)	8 Ocho.	Ofic.	R 99999	02/07/05
QUIMICA (05)(CBC)	9 Nueve.	Ofic.	R 99999	25/11/05
ALGEBRA (27)(CBC)	10 Diez.	Ofic.	R 99999	25/11/05
INT.PENSAMIENTO CIENTIFICO (40)(CBC)	7 Siete.	Ofic.	R 99999	25/11/05
LABORATORIO 1	10 Diez.	Ofic.	A 1578	24/07/06
FISICA 1	8 Ocho.	Ofic.	A 3232	26/12/06
MATEMATICA 1	9 Nueve.	Ofic.	A 162	20/02/07
MATEMATICA 3	8 Ocho.	Ofic.	A 504	13/03/07
LABORATORIO 2	10 Diez.	Ofic.	A 2267	24/07/07
FISICA 3	8 Ocho.	Ofic.	A 2206	13/08/07
LABORATORIO 3	10 Diez.	Ofic.	A 2925	13/12/07
FISICA 2	8 Ocho.	Ofic.	A 3433	27/12/07
MECANICA CLASICA	10 Diez.	Ofic.	A 340	21/02/08
LABORATORIO 4	10 Diez.	Ofic.	A 1347	16/07/08
FISICA 4	6 Seis.	Ofic.	A 3402	30/12/08
MATEMATICA 4	10 Diez.	Ofic.	A 50	24/02/09
LABORATORIO 5	10 Diez.	Ofic.	A 1552	05/08/09
ESTRUCTURA DE LA MATERIA 4	10 Diez.	Ofic.	A 3440	30/12/09
LABORATORIO 6	10 Diez.	Ofic.	A 4373	19/03/10
INCERTEZAS EXPERIMENTALES Y TEORIA DE ERR	9 Nueve.	Ofic.	A 1844	23/06/10
CALCULO NUMERICO	9 Nueve.	Ofic.	A 4170	28/12/10
LABORATORIO 7	10 Diez.	Ofic.	A 1551	24/06/11
DINAMICA NO LINEAL	10 Diez.	Ofic.	A 2046	08/08/11
FISICA TEORICA 1	10 Diez.	Ofic.	A 3047	28/10/11
ESTRUCTURA DE LA MATERIA 1	10 Diez.	Ofic.	A 3965	22/12/11
FISICA TEORICA 3	9 Nueve.	Ofic.	A 1476	08/06/12
FISICA TEORICA 2	10 Diez.	Ofic.	A 2599	28/09/12
ESTRUCTURA DE LA MATERIA 3	9 Nueve.	Ofic.	A 3665	27/12/12
RELATIVIDAD GENERAL	10 Diez.	Ofic.	A 1450	04/07/13
ESTRUCTURA DE LA MATERIA 2	7 Siete.	Ofic.	A 92	12/02/14
TESIS DE LICENCIATURA	10 Diez.	Ofic.	A 664	28/03/14

Materias Rendidas : 33 (treinta y tres)
Materias Aprobadas: 33 (treinta y tres)

A su pedido y al solo efecto de ser presentado ante las autoridades Nacionales Provinciales, Particulares y/o Extranjeras que lo soliciten, expido el presente en la Ciudad de Buenos Aires, a 27 días del mes de mayo de 2014.----------

María Delia Guy de Rey
Jefe de Departamento
Dirección de Alumnos y Graduados

University of Buenos Aires

Faculty of Exact and Natural Sciences

Academic Transcript

The one subscribing this document certifies that the record number: L 184/06 corresponding to Mr. Kevin Speyer student of Physical Sciences has taken the exams listed below:

Course	Description	Final Grade	Date (D/M/Y)
Physics (CBC*)	Elementary Mechanics	7	02/07/05
Introductory Notions on Society and State (CBC*)	History of XX century	8	02/07/05
Calculus (CBC*)	Introduction to differential Calculus	8	02/07/05
Chemistry (CBC*)	Basic Chemistry	9	25/11/05
Linear Algebra (CBC*)	Introduction to Linear Algebra	10	25/11/05
Introduction to Scientific Thought (CBC*)	Epistemology	7	25/11/05
Laboratory 1	Experimental Mechanics	10	24/07/06
Physics 1	Introduction to Classical Mechanics	8	26/12/06
Mathematics 1	Multivariate Calculus	9	20/02/07
Mathematics 3	Differential Calculus	8	13/03/07
Laboratory 2	Experimental Waves and Optics	10	24/07/07
Physics 3	Introduction to Electromagnetism	8	13/08/07
Laboratory 3	Experimental Electromagnetism	10	13/12/07
Physics 2	Introduction to Waves and Optics	8	27/12/07
Classical Mechanics	Classical Mechanics	10	21/02/08
Laboratory 4	Advanced Laboratory	10	16/07/08
Physics 4	Introduction to Thermodynamics and Quantum Physics	6	30/12/08
Mathematic 4	Complex Calculus	10	24/02/09
Laboratory 5	Advanced Laboratory	10	05/08/09
Structure of Matter 4	Particle and Nuclear Physics	10	30/12/09
Laboratory 6	Curricular Internship in a Laboratory	10	19/03/10
Incertezas Experimentales y Teoría de Errores	Probability and Statistics	9	23/06/10
Numerical Analysis	Numerical Analysis	9	28/12/10
Laboratory 7	Curricular Internship in a Laboratory	10	24/06/11
Nonlinear Dynamics	Nonlinear Dynamics	10	08/08/11
Theoretical Physics 1	Electromagnetism	10	28/10/11
Structure of Matter 1	Fluid Dynamics	10	22/12/11
Theoretical Physics 3	Statistical Mechanics	9	08/06/12
Theoretical Physics 2	Quantum Mechanics	10	28/09/12

Structure of Matter 3	Molecular Dynamics	9	27/12/12
General Relativity	General Relativity	10	04/07/13
Structure of Matter 2	Condensed Matter Physics	7	12/02/14
Thesis[1]	MS Dissertation	10	28/03/14

Courses Attended: 33
Courses Approved: 33

At your order and for the sole purpose of being presented to the National, Provincial, Particular and/or Foreigners authorities, I issue this certificate in the Autonomous City of Buenos Aires, being the 27th of May of 2014.

Faculty of Natural Sciences
University of Buenos Aires

Maria Delia Guy de Rey
Students and Graduates Office

1 Translator's Note:

*CBC is the Common Basic Cycle of the University of Buenos Aires, equivalent to a mandatory Foundation Year

Candidate Average: 9.06 (with CBC) 9.26 (without CBC) out of 10
Faculty Average: 8.48 (with CBC) 8.73 (without CBC) out of 10
1 being the lowest grade and 10 the maximum grade.

Ministerio de Ciencia, Tecnología e Innovación Productiva
Consejo Nacional de Investigaciones Científicas y Técnicas

----------CERTIFICO que el Licenciado **SPEYER, KEVIN (DNI N° 33.023.577),** es Becario de este Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) en la categoría de Beca Interna Doctoral, otorgada por Resolución D N° 4860 de fecha 17 de Diciembre de 2013, desde el 01 de Abril de 2014 hasta el 31 de Marzo de 2019; período en el cual desarrolla tareas de investigación sobre el tema: "**Estudio por simulación del flujo de líquidos con finados por cepillos poliméricos semiflexibles**" bajo la dirección del Doctor **PASTORINO, CLAUDIO** en el **GERENCIA FISICA (CAC); GERENCIA D/AREA INVEST Y APLICACIONES NO NUCLEARES; COMISION NACIONAL DE ENERGIA ATOMICA**----------

----------En su carácter de Becario Interno Doctoral, el Licenciado **SPEYER, KEVIN (DNI N° 33.023.577),** percibe un estipendio mensual de **PESOS CATORCE MIL CIENTO VEINTISIETE CON VENTICUATRO CENTAVOS ($14.127,24)**----------

----------A solicitud del interesado y para ser presentado ante quien corresponda, se extiende el presente certificado en la Ciudad de Buenos Aires, al día 03 de agosto de 2016----------

CONSEJO NACIONAL DE INVESTIGACIONES CIENTÍFICAS Y TÉCNICAS - Ministerio de Ciencia, Tecnología e Innovación Productiva

Gimena RIVERO
Jefa Depto. de Becas
CONICET

Scholarship Certificate

Ministry of Science, Technology and Productive Innovation
National Scientific and Technical Research Council (CONICET)

I certify that the Licentiate Kevin Speyer (National identity document number 33023577), has been awarded a PhD scholarship, by the National Scientific and Technical Research Council, resolution number 4860 on the 17th of December of 2013, from the 1st of April of 2014 to 31st of March 2019. In this period he will be performing research tasks on the topic: “Simulations of liquid flow confined by semiflexible polymer brushes” supervised by Dr. Claudio Pastorino in the Physics Department of the Constituyentes Atomic Center (CAC); Managment area of non nuclear research and application, National Atomic Energy Commission (CNEA).

In Accordance to his PhD Candidate position, the Licenciate Kevin Speyer receives a monthly scholarship amount of $14.127,24 Argentinean Pesos.

Written upon request, and to be presented to the corresponding authorities, this certificate is emitted in the City of Buenos Aires, on the 3rd of August of 2016.

Gimena Rivero
Chief of the Scholarship Department
CONICET