

Exploring the Physics of Small Devices

Programme Acronym EPSD

Standing committee PESC

Principal Applicants

Christian Van den Broeck (contact person)

Dept WNI, Hasselt University, Agoralaan, B-3590 Diepenbeek, Belgium

Tel 3211268214 Fax 3211268299

christian.vandenbroeck@uhasselt.be

Juan MR Parrondo

Dep. Física Atómica, Molecular y Nuclear, Universidad Complutense de Madrid

Ciudad Universitaria s/n, 28040 Madrid Spain

Tel: +34 91 394 4741 Fax: +34 91 394 5193

parrondo@fis.ucm.es

<http://seneca.fis.ucm.es/parr>

Udo Seifert

 Institut fuer Theoretische Physik, Universitaet Stuttgart

Pfaffenwaldring 57, 70550 Stuttgart, Germany

Tel: ++ 49 711 685-64927 Fax: +49 711 685 64902

useifert@theo2.physik.uni-stuttgart.de

<http://www.theo2.physik.uni-stuttgart.de/institut/seifert/seifert.html>

Keywords

Nonequilibrium nanodevices, stochastic thermodynamics, control and efficiency, molecular engines.

Abstract

Our network joins leading European laboratories at the forefront of experimental studies of small physical, biophysical and chemical devices, to the theoretical groups that have pioneered recent spectacular advances in the nonequilibrium physics of small systems. Such a unique cross-disciplinary network will push forward the integration between theory, experiment and application, allow to solve technical problems specific for the small scale and inspire new methods of design, manipulation and operation. We will further develop and apply the thermodynamics and statistical mechanics of small nonequilibrium devices, evaluate the role of stochasticity and nonlinearity and the implementation of optimization techniques, and develop new calculational approaches for small driven systems. Important inspiration will also be drawn from the incorporation of groups working on the physical understanding of biological machines like molecular motors and other "devices" operating in the cell and their corresponding biotechnological applications. The implications of these new theoretical and conceptual perspectives will be confronted with the practical and technological issues posed by the design and construction of small scale devices, in synergy with the participating research laboratories working on nanoelectronics, nanorefrigeration, supra-molecular devices, catalytic devices, biotechnology of the cell, micro-fluidics and micro-arrays. We will also devote special attention to expertise-broadening training of young scientists.

Proposal

1. Status

Recent technical, experimental, conceptual and theoretical advances open new perspectives, not only for the study or understanding of small systems, but also for their manipulation, control and manufacture. The theoretical breakthroughs offer a new vision on the relation between the micro and macro worlds, in particular the impact of dynamical randomness, the relationship between fluctuations, entropy production and work, and the role of stochasticity in small scale non-linear nonequilibrium phenomena. On the conceptual side, rather than miniaturizing the construction and principles of macroscopic machines, one can build on the specificities of the small scale such as the presence of a strong stochastic component, to propose new designs and new modes of operation. Advances in the study, measurement, manipulation or even manufacture of small devices are even more spectacular. The technical and experimental breakthroughs include a whole array of new measuring, manufacturing and controlling devices such as atomic force microscopy, scanning probe microscopy, field emission microscopy, optical tweezers etc., an array of techniques from lithography, biotechnology and supra-molecular chemistry, and many new and improved methods developed in nanotechnology (nanoelectronics, nanomedicine, nanotubes, micro-fluids, etc.).

2. Motivation and Plus Value

Our network offers a unique expertise spanning the whole range from purely theoretical research to experimental and applied research. The majority of the laboratories are in fact involved in experimental research, while the theoretical groups are at the forefront of the recent developments concerning the physics of small devices. Topics include: nonequilibrium statistical mechanics, stochastic processes, stochastic thermodynamics, non-linear dynamics, numerical techniques, control theory, pattern formation, supra-molecular chemistry, nanoelectronics and nanomaterials, charge transport and thermal properties in nano- and microstructures, biotechnology of small devices, catalysis at the nanoscale, experimental and theoretical biophysics of the cell. In fact, each of the participating groups has performed pioneering work in one or several of the above mentioned topics. Nevertheless, in the absence of a common structure or overarching network, and due to the involvement of different scientific communities, chemical, biological, physical and engineering science, the cross-interactions have been relatively limited.

Previous experience has shown that such contacts can lead to genuine new ideas. As concrete examples of such cross-fertilization, some of which were generated by incidental contacts in the StochDyn ESF network, we cite new computation techniques for free energy estimation, Brownian refrigerator in nanosuperconductors, issues of Carnot efficiency for Brownian motors in supra-molecular chemistry, various proposals for micro-sieves and other micro-fluidic devices.

The main strategic purpose of the network will be to organize such cross-disciplinary contacts on a more systematic basis and centered around specific problems suggested by either the participating theoretical or experimental groups. Equally important, the network will allow to expose young researchers on the level of a European network of excellence to expertises that cross the traditional boundaries between disciplines. As far as

the scientific aspect is concerned, the topics on which we will focus are expounded in more detail below.

3. Theory: Concepts, Techniques and Perspectives

Since the 1990s several European groups have booked major advances in the theoretical and conceptual description of small systems. One class of results is related to what is usually referred to as fluctuation and work theorems. These results extend the pioneering work of Onsager to far from equilibrium situations. They can be derived at the Hamiltonian level and provide a new foundation for the second law and the interpretation of irreversibility [VandenBroeck1], and can also be formulated more generally for dynamical systems [Gaspard].

When operating at a mesoscopic scale, relevant for some physical and chemical and most biophysical applications, a new field called “stochastic thermodynamics” or “path thermodynamic” has been developed [Seifert1, Peliti] This approach generalizes the classical concepts of thermodynamics to small driven systems by assigning a weight to each phase-space path. Exact results for the distribution of work and entropy production can be derived. In some cases, dynamical phase transitions may occur which are associated with exponential tails in the work or entropy flow distributions. Since successful comparisons with experimental model systems have proven the fundamental potency of this new framework [Seifert2], it can and should now be applied to both more complex biological systems and technologically relevant devices.

The concept of thermodynamic stability and, in particular of a phase transition itself, has to be revisited when dealing with small systems. When discussing structural and morphological phase transitions in nanoparticles, one has to realize that the physical and chemical properties can change dramatically essentially due to the large surface to volume ratio. Transformation pathways blocked in the macroscopic material might become favored in the nanoparticle, because they lead to shapes with particularly low surface free energies. Also, thermal fluctuations, which affect the stability of nanoparticles, are of increasing importance as size is scaled down. In view of the possible use of such nanoscale systems as building blocks for novel devices, understanding these effects on an atomistic level is of fundamental importance [Dellago1].

Another question related to pattern formation deals with the combination of external fields with fluctuations in the formation of e.g. precipitation patterns. A deeper understanding will help the design of noise-controlled patterns on micro- and nanoscales [Racz].

Specific concepts from the field of stochastic processes open novel perspectives in the study of various small scale phenomena, including electron transfer theory, the modeling of simple molecular wires based on the structure of DNA, studies of electronic properties of random polymers, and the investigation of radiation-induced fragmentation processes in DNA. In particular, the analysis of spectral diffusion in single molecule spectroscopy relates to a class of generalized Markovian processes with stable (Lévy) distribution of increments. Such models also describe the stochastic dynamics of particles or excitations moving along fastly folding polymers [Gudowska].

4. Devices: Physical

The appearance of fluctuations in small systems has led to new concepts for characterizing or operating such devices, exploiting rather than fighting these very same fluctuations. We cite the principles of Brownian motors [Prost1], stochastic resonance and resonant activation, Brownian refrigerator [VandenBroeck2], stochastic synchronization, Parrondo paradox [Parrondo] and free energy estimations from fluctuations [Dellago2]. The basic question about the efficiency of the devices has to be re-examined [Parrondo1]. For operation far from equilibrium, one can wonder whether the efficiencies predicted close to thermodynamic equilibrium, such as the Carnot and Curzon-Ahlborn efficiency, can be reached. In particular it appears that very high efficiencies are attained in biological motors. The understanding of these mechanisms from the new theoretical perspectives has obviously great technological potential. Besides the direct application to thermally, optically or chemically driven nanomotors [Gaub], these insights can guide the design for nanoversions of the refrigerator, the thermo-couple, the Peltier element and the photovoltaic cell.

Concerning electro-thermal or electro-optical processes, we mention the charge transport and thermal properties in nano and microstructures [Pekola]. The interplay of the various relaxation rates and the energy filtering of electrons in superconducting-metal structures opens a very versatile and well controlled domain for studies of thermal phenomena in nanosized structures and devices. These include quantized thermal conductance by photons, cyclic electronic refrigeration utilizing single-electron charging effect and energy filtering, and Brownian refrigeration of electrons.

The interplay between fluctuations, disorder, and collective phenomena can also be observed in micro- and nanostructured materials fabricated by means of lithographic techniques. A rich phenomenology of ratchet effects has been observed for fluxons in superconducting films [Vicent] and also in the motion of domain walls in magnetic materials [Parrondo2], providing new design strategies for nanodevices.

The effect of noise (chiefly non-white noise) upon oscillators, with particular emphasis on phase noise-induced frequency shifts, is relevant in models of micro-electronic oscillators and phase-locked loops [Gleeson].

5. Devices: Biophysical

From a biophysical perspective, the fundamental constituents of the cell like membranes, proteins and molecular motors and their cooperative action in essential functions of cell life like intracellular traffic, adhesion, dynamics and motility, signal transduction and sound detection are modelled and studied both experimentally and theoretically using these novel concepts from non-equilibrium statistical mechanics [Prost2]. Inside cells, molecular motors can act individually for example to transport material along filaments, but they often act collectively, as in muscles, in some cells to provoke the beating of cilia, or in the cytoskeleton where they create internal contractile stresses and active fluctuations. The behavior of single motors is well understood in terms of two-level systems or Brownian ratchets. The collective behavior of molecular motors is less understood and in general leads to dynamic phase transitions, instabilities, and oscillatory behavior [Prost1]. The study of specific cases in cell biology provides a challenging application of physics at a small scale. With regard to the hair cells, recent biomimetic experiments

with actin filaments can be reproduced well by the non-linear force displacement relation of the hair cell cilia. Myosin motors on the other hand confer to the cytoskeleton an active character: the cytoskeleton is maintained in a nonequilibrium state because of the constant consumption of energy of the molecular motors. Models to describe active polar gels and more generally the statistical physics of active materials have recently been proposed but many properties of the cytoskeleton such as the non-equilibrium noise or the finite frequency rheology remain to be understood [Julicher].

Molecular motors seem to be remarkably efficient despite the fact that they operate far from equilibrium. If the principles uncovered in such studies can be transferred to new technological problems like transport, separation and sorting of nano and micro-particles, e.g. by using micro-scale particle sorters and optical lattice-based devices, a major technological spin-off can be achieved.

As a related application from the area of biotechnology, micro-arrays have become a powerful tool to monitor the gene expression level of thousands of genes simultaneously on a genome-wide scale. In these devices, RNA targets in solution bind to surface-bound DNA probes, and a marker makes the RNA/DNA complex fluorescent. The intensity measured from a specific spot on the microarray, with a specific DNA sequence, reflects the concentration of the complementary RNA. A quantitative estimation of the RNA concentration hinges on the relation between fluorescent intensity and concentration. These effects can be accessed with the combination of biochemistry (the various binding free energies) and statistical physics (the partition sum over all possible ways in which two strands can bind to each other) [Barkema].

6. Devices: Chemical

Some of the recent advances of synthetic chemistry also require a theoretical framework based on the physics of small systems. Chemists have demonstrated imagination and considerable skill in the design and construction of synthetic molecular systems in which positional displacements of submolecular components result from moving downhill in terms of energy [Leigh]. But what are the structural features necessary for molecules, which are undergoing incessant Brownian motion, to repetitively do mechanical work? How can we make a molecular machine that pumps ions to reverse a concentration gradient, for example, or moves itself uphill in terms of energy? How can we make nanoscale structures that traverse a predefined path across a surface or down a track by responding to the nature of their environment so as to change direction? How can we make a synthetic molecular motor that rotates against an applied torque?

Artificial compounds that can do such things have yet to be realized. However, the fundamental guidelines necessary to invent them are being studied by physicists. A close interaction between chemists and physicist is needed to understand how these often theoretical ideas can be implemented into actual synthetic molecular structures to create working experimental artificial molecular machines. The network will promote such collaboration to explore the possibility of producing experimental examples of some or all of the following types of mechanism: flashing ratchets, tilting ratchets, Seebeck ratchets, drift ratchets, Hamiltonian ratchets, temperature ratchets, and entropic ratchets.

Catalysis is another immensely important field of research, for which the understanding of the interplay between physics and chemistry at the very small scale is essential. In

field emission microscopy, atoms at the tip are ionized by a high electric voltage, allowing to observe crystal facets and their dynamics at the nanoscale. This technique is used to study chemical reactions of heterogeneous catalysis with nanometric resolution. In particular, oscillating chemical reactions have been observed in the reduction of NO_2 with H_2 on platinum or in the $\text{O}_2 + \text{H}_2$ reaction forming water on rhodium. These systems are typical out-of-equilibrium nanosystems. The understanding of these processes at the nanoscale remains an open problem, with obvious technological implications for the construction of catalytic devices [Kruse].

7. Synopsis

This network takes on the challenge to forge closer ties between leading theoretical, experimental and technological laboratories in the area of small nonequilibrium physical, biophysical and chemical devices. This extremely promising field of research is evolving at an unprecedented pace. We should not miss an opportunity to fuse the European expertise in a field that will play an important role in the technology of the 21st century.

8. References

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Facilities

The participating laboratories offer a wide and extensive array of facilities for experimental, theoretical and numerical research. Several of them dispose of appropriate logistics with tested experience for organizing workshops and conferences.

Benefit European Collaboration

The mobility of research, academic resources and human capital is still insufficient in Europe even in fields in which we have a very strong expertise as well as in those which have high technological promise. The mobility issue exists both in its geographical sense as in the sense of cross- and interdisciplinary collaboration. This lack of mobility is especially unfavorable in emerging fields such as the physics of small devices.

The first aim of our network will be to increase the mobility in the fields of research that are specified in the proposal. The network will join leading laboratories from 17 European countries, working in mathematics, physics, chemistry and biophysics and engineering, and using completely different technical, analytical and computational tools in their study of small devices. Many of the involved research groups, while very prominent in their specific own research field, have no active contacts with each other. We will forge personal collaboration, by strongly promoting the exchange of students, junior and

senior researchers in visits of short or medium duration. The organization of thematic meetings will allow to gather experts and students from different backgrounds around a common theme and provide a European forum for other researcher to join in. In particular, this will help to forge and strengthen crucial ties between the non-equilibrium mechanics and the nanodevices communities. We will initiate the process of mutual acquaintance in several steps. First we plan a meeting of the steering committee to get familiar with the mode of operation and discuss in more detail about start-up activities. This will include the planning for the first major event, namely an opening conference in which representatives of all the participating laboratories will expose their research topics and methods. Next, we will organize exploratory meetings followed later by thematic meetings, in which more specific collaboration around themes of common interest will be promoted. The groups not only differ in specific research interest but also in their involvement into basic or applied research. Our network will again try to bridge the gap, especially by promoting exchanges that join such laboratories.

Our second and even more important main goal is focused on the formation of students and junior researchers. While exchange of students between European laboratories is promoted through several European programs, our network will provide a sense of belonging to a broadly based high quality community of research centered on a theme that has both fundamental and technological appeal. It will allow contact with other groups, other than the natural partners of the home institution. We will encourage such collaboration by grants for visits of short and medium duration. Also we will organize two schools (introductory school in 2009 and a more advanced in 2011) providing intensive and extensive guided education into current topics of interest, with special attention to the bridging of disciplines and to the presentation of topics that are not treated in university curricula. These schools will be widely advertised and will obviously be open, and - within the limits of the budget - freely accessible to all students from participating European countries. Students will also receive substantial subsidies for participation in our other main events and a la carte for more specialized thematic meetings.

Our third and final aim will be to initiate or strengthen collaboration between laboratories that may be working on related subjects but have, for some reason, not been closely in touch with each other. This includes the connection between theoretical and more applied laboratories and to cross-disciplinary work. Exchange of students and researchers, the organization of specific thematic meetings and the very existence of the network should promote these contacts.

Proposed activities

The schedule of activities is schematically represented in the table below (assuming start of activities in 2009). We distinguish three main ingredients: a yearly main event (school or conference), smaller meetings (5-10 per year) and exchange visits by senior and junior researchers and by students (short and medium duration, total of about 40/year).

Duration: 60 months

Budget estimate 100 keuro/year total 500 keuro

Main event: 19.5 keuro/year

30+ participants 4-5 days

Conferences: 3 organizers + 7 speakers at 800 euro, 15 student grants at 600 euro and 2.5 keuro other expenses.

Schools: 6 speakers at 1000 euro, 15 student grants at 600 euro and 4.5 keuro other expenses.

The opening meeting will be combined with a first meeting of steering committee. The further distribution of the funds will be decided via email consultation.

Workshops: 36 keuro/year

3-12 keuro/meeting, 5 meetings per year

Researcher visits: 16 keuro/year

15 short time visits 800 euro/visit

4 long time visits 1000 euro/visit

Student visits: 14 keuro/year

15 short time visits 600 euro/visit

5 long time visits 1000 euro/visit

ESF administrative cost (14.5%) 14.5 keuro/year

2009	2010	2011	2012	2013
Opening Meeting	Introductory School	Conference	Advanced School	Closing Conference
Exploratory Meetings	Thematic Workshops	Thematic Workshops	Thematic Workshops	Satellite Meetings
Initiating Visits	Exchange Visits	Exchange Visits	Exchange Visits	Concluding Visits
Student Visits	Student Visits	Student Visits	Student Visits	Student Visits
85.5 keuro	85.5 keuro	85.5 keuro	85.5 keuro	85.5 keuro

Appendix 1: CV

Christian Van den Broeck.

Universiteit Hasselt B-3590 Diepenbeek Belgium

Education	Aggregation Higher Education Vrije Universiteit Brussel, Belgium	1989
	Ph. d. Physics Vrije Universiteit Brussel, Belgium	1980
	Licentiate Physics Rijksuniversiteit Gent, Belgium	1976
Academic Position (Main Track)	Full Professor (BOF research chair) Universiteit Hasselt, Belgium	2003-present
	Associate Professor (BOF research chair) Limburgs Universitair Centrum, Belgium	2000-2003
	Researcher (tenured, senior and director) F. W. O.-Vlaanderen	1985-2000

Other academic information

170 papers in refereed journals, 2500 citations, co-editor Europhysics Letters, Noise and Fluctuations Letters, Organizer of 9 workshops and conferences over past 10 years, co-chair Stochdyn program ESF/PESC 2003-2008, local chair of 3 programmes of excellence (IUAP) of the Belgian government, frequently invited speaker at conferences (10X/year) and universities (5X/year).

Five recent publications

C. Van den Broeck, "Thermodynamic Efficiency at Maximum Power", Phys. Rev.Lett. **95**, 190602 (2005); B. Cleuren, C. Van den Broeck and R. Kawai, "Fluctuation and Dissipation of Work in a Joule experiment", Phys. Rev. Lett. **96**, 050601 (2006); K. Wood, C. Van den Broeck, R. Kawai and K. Lindenberg, "Universality of Synchrony: Critical Behavior in a Discrete Model of Stochastic Phase-coupled Oscillators", Phys. Rev. Lett. **96**, 050601 (2006); C. Van den Broeck and R. Kawai, "Brownian Refrigerator", Phys. Rev. Lett. **96**, 210601 (2006); R. Kawai, J.M.R. Parrondo and C. Van den Broeck, "Dissipation: The Phase-Space Perspective", Phys. Rev. Lett. **98**, 080602 (2007).

Juan MR Parrondo.

Universidad Complutense de Madrid. 28040-Madrid, Spain

Education	Ph. D. Physics Universidad Complutense de Madrid	1992
	Licentiate Physics Universidad Complutense de Madrid	1987
Academic Position (Main Track)	Professor Universidad Complutense de Madrid	1996-present
	Assistant Professor Universidad Complutense de Madrid	1987-1996

Other academic information

50 papers in refereed journals, 900 citations, co-editor Noise and Fluctuations Letters, referee for national and international funding agencies; frequently invited speaker at conferences (5 /year).

Five recent publications

L. Dinis, E. M. Gonzalez, J. Anguita, J.M.R. Parrondo, and J.L. Vicent, "Lattice effects and current reversal in superconducting ratchets", *New J. Phys.* **9**, 366 (2007); R. Kawai, J.M.R. Parrondo and C. Van den Broeck, "Dissipation: The Phase-Space Perspective", *Phys. Rev. Lett.* **98**, 080602 (2007); L. Dinis, J.M.R. Parrondo, and F.J. Cao. "Closed-loop control strategy with improved current for a flashing ratchet" *Europhys. Lett.* **71**, 536 (2005); F. Cao, L. Dinis, and J.M.R. Parrondo, "Feedback control in a collective flashing ratchet", *Phys. Rev. Lett.* **93**, 040603 (2004); J.M.R. Parrondo and L. Dinis, "Brownian motion and gambling: from ratchets to paradoxical games", *Contemp. Phys.* **45**, 147 (2004).

Udo Seifert

Universität Stuttgart, D-70550 Stuttgart, Germany

Education	Habilitation in Theoretical Physics Ludwig-Maximilians-Universität München	1995
	Ph. D. Physics Ludwig-Maximilians-Universität München	1989
	Physics Diploma Ludwig-Maximilians-Universität München	1985
Academic Position	Full Professor for Theoretical Physics Universität Stuttgart	2001-present
	Staff Scientist Max Planck Institute for Colloids & Interfaces, Potsdam	1995-2001
	Research Fellow Research Centre, Jülich	1993-1994
	Post-Doc Simon Fraser University, Vancouver, Canada	1990-1992

Other academic information :

90 papers in refereed journals, 2500 citations; Divisional Associate Editor *Physical Review Letters*; Co-Editor *Europhysics Letters*; Referee for national and international funding agencies; member of the steering committee of the priority program "Microfluidics" of the German science foundation (2004-2008); frequently invited speaker to colloquia and conferences (> 10 / year).

Five recent publications:

T. Schmiedl and U. Seifert, "Optimal finite-time processes in stochastic thermodynamics", *Phys. Rev. Lett.* **98**, 108301 (2007); V. Blickle, T. Speck, C. Lutz, U. Seifert, and C. Bechinger, "Einstein relation generalized to nonequilibrium", *Phys. Rev. Lett.* **98**, 210601 (2007); V. Blickle, T. Speck, L. Helden, U. Seifert, and C. Bechinger, "Thermodynamics of a colloidal particle in a time-dependent non-harmonic potential", *Phys. Rev. Lett.* **96**, 070603 (2006); U. Seifert, "Entropy production along a stochastic trajectory and an integral fluctuation theorem", *Phys. Rev. Lett.* **95**, 040602 (2005); S. Schuler, T. Speck, C. Tietz, J. Wrachtrup, and U. Seifert. "Experimental test of the fluctuation theorem for a driven two-level system with time-dependent rates", *Phys. Rev. Lett.* **94**, 180602 (2005).

Appendix 2: Steering committee

<p>Austria Christoph Dellago Faculty of Physics, University of Vienna Boltzmannngasse 5 1090 Wien, Austria Tel: +43 1 4277 51260 Fax: +43 1 4277 9511 Christoph.Dellago@univie.ac.at</p>	<p>Belgium (Flemish) Christian Van den Broeck (contact person) Hasselt University Agoralaan B-3590 Diepenbeek, Belgium Tel: +32 11268214 Fax: +32 11268299 christian.vandenbroeck@uhasselt.be</p>
<p>Belgium (French) Pierre Gaspard Service de Chimie Physique CP231 Universite Libre de Bruxelles Campus Plaine Bd. du Triomphe B-1050 Bruxelles, BELGIUM Tel: +32 2 650 57 93 Fax: +32 2 650-5767 gaspard@ulb.ac.be</p>	<p>Denmark Henrik K. Flyvbjerg Biosystems department BIO-313 P.O. Box 49 Risø National Laboratory Frederiksborgvej 399 DK-4000 Roskilde, Danmark 05 Tel: +45 4677 4104 henrik.flyvbjerg@risoe.dk</p>
<p>Finland Jukka Pekola Low Temperature Laboratory Helsinki University of Technology Micronova, Tietotie 3, office 4110 P.O. Box 3500, 02015 TKK, Finland Tel: +35 8 9 4514913 Fax: +35 8 9 451 5008 jukka.pekola(at)tkk.fi</p>	<p>France Jacques Prost Curie Institute Research Center 26 rue d'Ulm, 75248 Paris cedex05, France and ESPCI 10 rue Vauquelin, 75231 Paris ce- dex05, France Tel: +33 140794500 Fax:+33 145351474 Jacques.prost@curie.fr</p>
<p>Germany Udo Seifert II .Institut fuer Theoretische Physik Universitaet Stuttgart Pfaffenwaldring 57, 70550 Stuttgart, Germany Tel: +49 711 685 64927 Fax: +49 711 685 64902 useifert@theo2.physik.uni-stuttgart.de http://www.theo2.physik.uni-stuttgart.de/institut/seifert/seifert.html</p>	<p>Great Britain David A Leigh School of Chemistry, University of Edinburgh The King's Buildings, West Mains Road, Edinburgh EH9 3JJ, United Kingdom Tel: +44 131 650 4730 (Secretary) or 650 4721 Fax: +44 131 650 6453 David.Leigh@ed.ac.uk http://www.catenane.net</p>
<p>Hungary Zoltan Racz Institute for Theoretical Physics Eotvos University, Pazmany s. 1/a 1117 Budapest, Hungary Tel: +36 1 372 2516 Fax: +36 1 372 2509 racz@general.elte.hu</p>	<p>Ireland James Gleeson Department of Mathematics and Statistics University of Limerick Limerick, Ireland Tel: +35 361 202634 Fax: +35 361 334859 james.gleeson@ul.ie</p>

<p>Italy Luca Peliti Dipartimento di Scienze Fisiche Università "Federico II" Complesso Monte S. Angelo I-80126 Napoli (Italy) Tel. and Fax: +39 081 676 479 http://people.na.infn.it/~peliti</p>	<p>Netherlands Gerard T. Barkema Institute for Theoretical Physics Leuvenlaan 4 3584 CE Utrecht, Netherlands Tel.: +31 30 253 2954 Fax : +31 30 253 5937 Barkema@phys.uu.nl http://www.phys.uu.nl/~barkema/</p>
<p>Norway Alex Hansen Department of Physics Norwegian University of Science and Technology N-7491 Trondheim Norway Tel.: + 47 73 53 77 10. Fax.:+ 47 73 59 77 10 Alex.Hansen@ntnu.no</p>	<p>Poland Ewa Gudowska-Nowak M. Smoluchowski Institute of Physics Jagellonian University, ul. Reymonta 4 30-059 Krakow, Poland Tel.: +48 12 663 5567 Fax.: +48 12 633 4079 gudowska@th.if.uj.edu.pl http://th-www.if.uj.edu.pl/zfs/gudowska/gucia.html</p>
<p>Portugal José Luís da Silva Mathematics and Engineering Depart- ment (CCM), University of Madeira Campus da Penteada 9000-390 Funchal, Madeira, Portugal Tel: +35 1 291 705185 Fax: + 35 1 291 705189 luis@uma.pt</p>	<p>Spain Juan MR Parrondo Dep. Física Atómica, Molecular y Nuclear Universidad Complutense de Madrid, Spain Tel: +34 91 394 4741 Fax: +34 91 394 5193 parr@seneca.fis.ucm.es http://seneca.fis.ucm.es/parr</p>
<p>Sweden Hongqi Xu Mesoscopic Physics and Nano Devices Division of Solid State Physics Lund University, Box 118 S-221 00 Lund Sweden Tel: + 46 46 222 7759 Fax: + 46 46 222 36 Hongqi.Xu@ftf.lth.se http://www.ftf.lth.se; http://nano.lth.se</p>	<p>Switzerland Max-Olivier Hongler Doctoral program "Production and Robotics" STI/IPR/LPM (station 17) Ecole Polytechnique Fédérale de Lau- sanne(EPFL) CH-1015 Lausanne, Switzerland Tel: +41 21 693 5391 Fax: +41 21 693 3891 max.hongler@epfl.ch</p>

Appendix 3: Programme collaboration

Below we give a short list of laboratories that explicitly endorse our proposal.

<p>Belgium (Flemish) Francois Peeters University of Antwerp Condensed Matter Theory Department of Physics (U213) Groenenborgerlaan 171 B-2020 Antwerpen, Belgium francois.peeters@ua.ac.be</p>	<p>Belgium (French) Norbert Kruse Chimie Physique des Matériaux Université Libre de Bruxelles, Campus Plaine, CP243, Bd. du Triomphe B-1050 Bruxelles, Belgium nkruse@ulb.ac.be</p>
<p>France Sergio Ciliberto Laboratoire de Physique ENS de Lyon 46 Allée d'Italie 69364 Lyon, France sergio.ciliberto@ens-lyon.fr</p>	<p>Germany Hermann Gaub LMU München Lehrstuhl für angewandte Physik Amalienstr. 54 80799 München, Germany gaub@physik.uni-muenchen.de</p> <p>Peter Hanggi Institut für Physik Universität Augsburg Universitätsstr. 1 D-86135 Augsburg, Germany hanggi@physik.uni-augsburg.de</p>
<p>Italy Fabio Marchesoni Department of Physics University of Camerino I-62032 Camerino, Italy and INFN - VIRGO Project University of Perugia I-06123 Perugia, Italy fabio.marchesoni@pg.infn.it</p>	<p>Netherlands Daan Frenkel FOM-Institute for Atomic and Molecular Physics [AMOLF] Kruislaan 407, 1098 SJ Amsterdam The Netherlands and Department of Chemistry University of Cambridge, Lensfield Road Cambridge CB2 1EW, UK frenkel@amolf.nl</p>
<p>Spain Felix Ritort Departament de Física Fonamental University of Barcelona Diagonal 647 08028 Barcelona, Spain ritort@correu.ffn.ub.es</p>	<p>Sweden Lars Samuelson Division of Solid State Physics Lund University Sölvegatan 14 S-223 62 Lund, Sweden Lars.Samuelson@ftf.lth.se</p>